

FIG.1

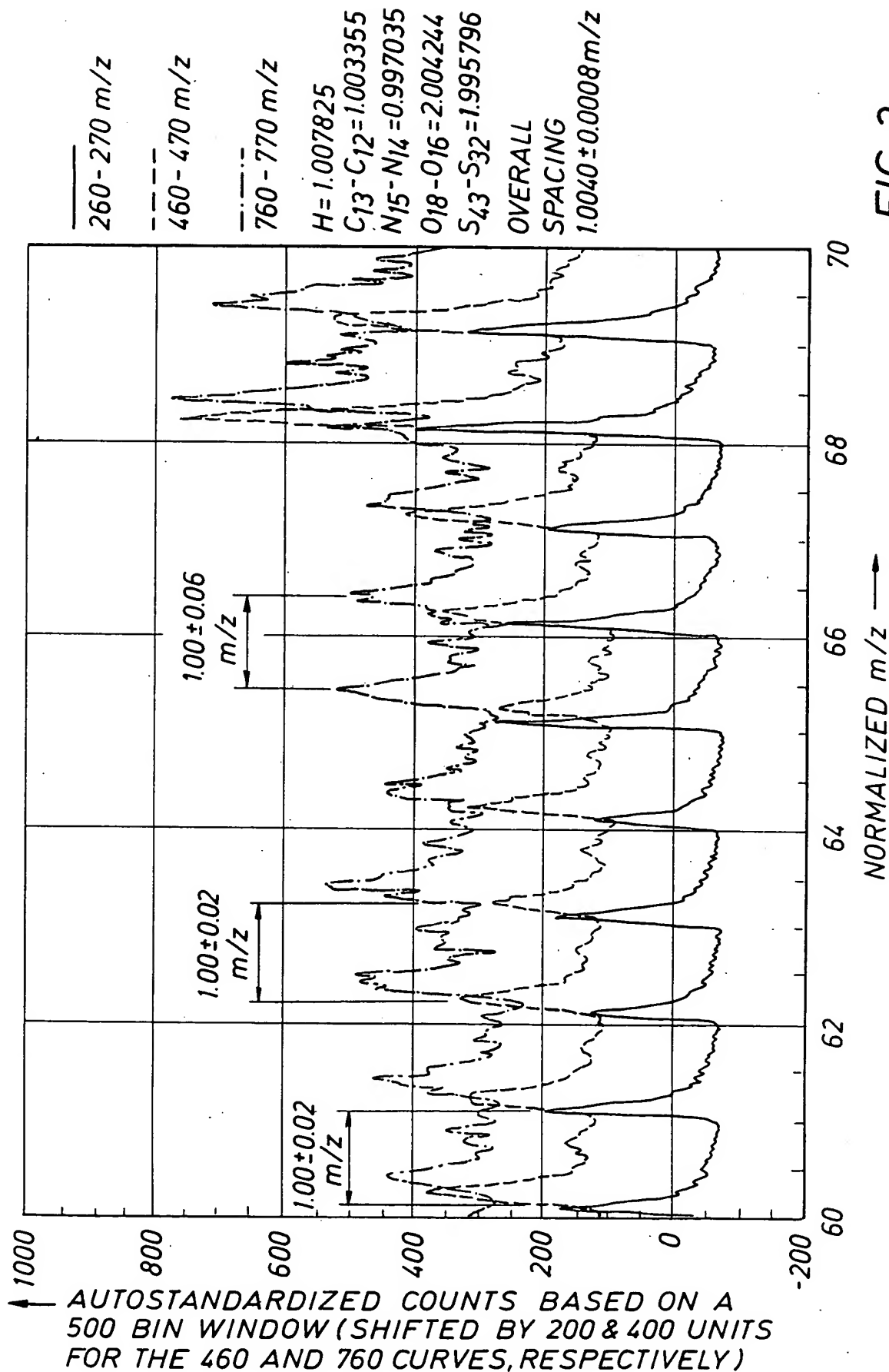
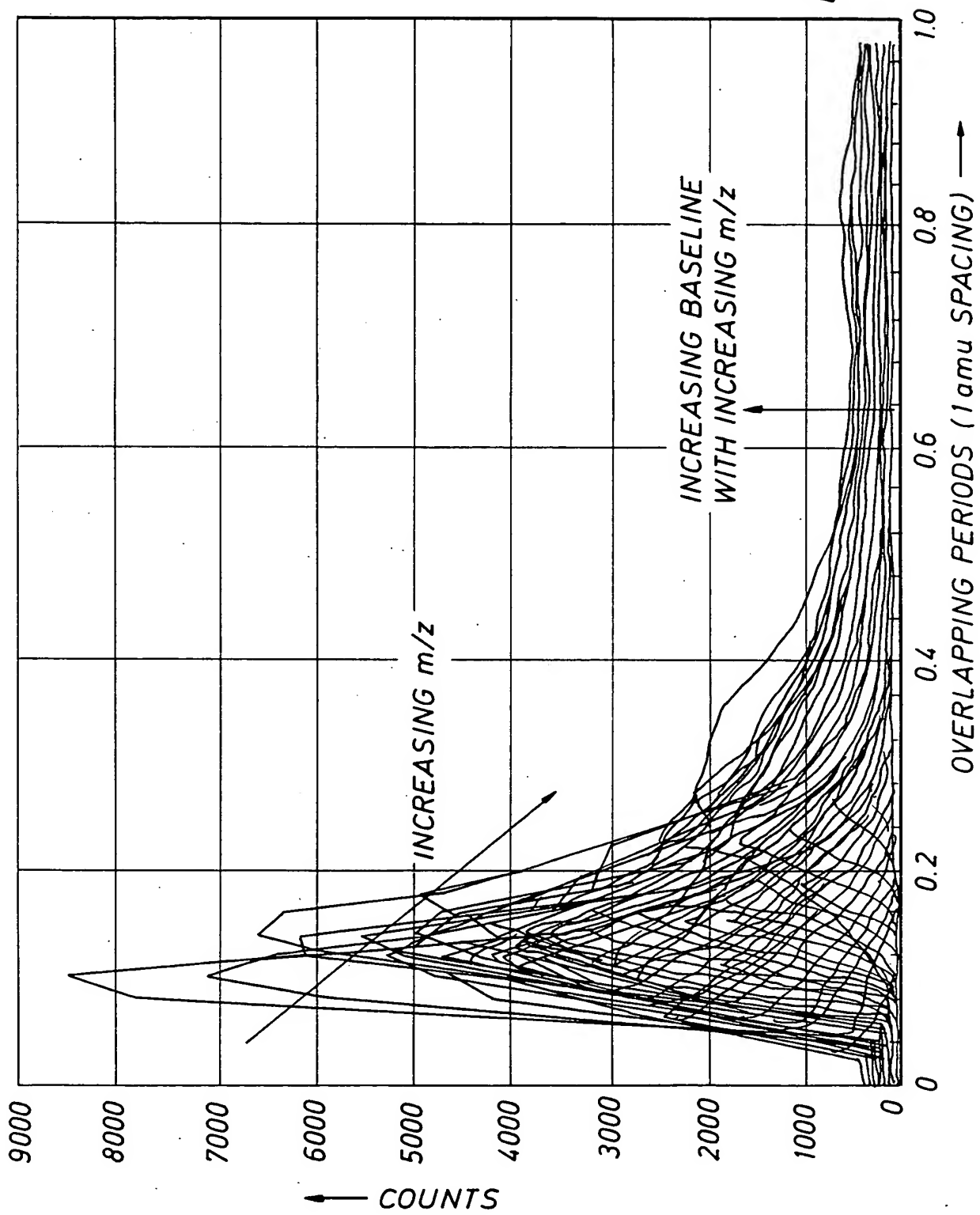


FIG. 2



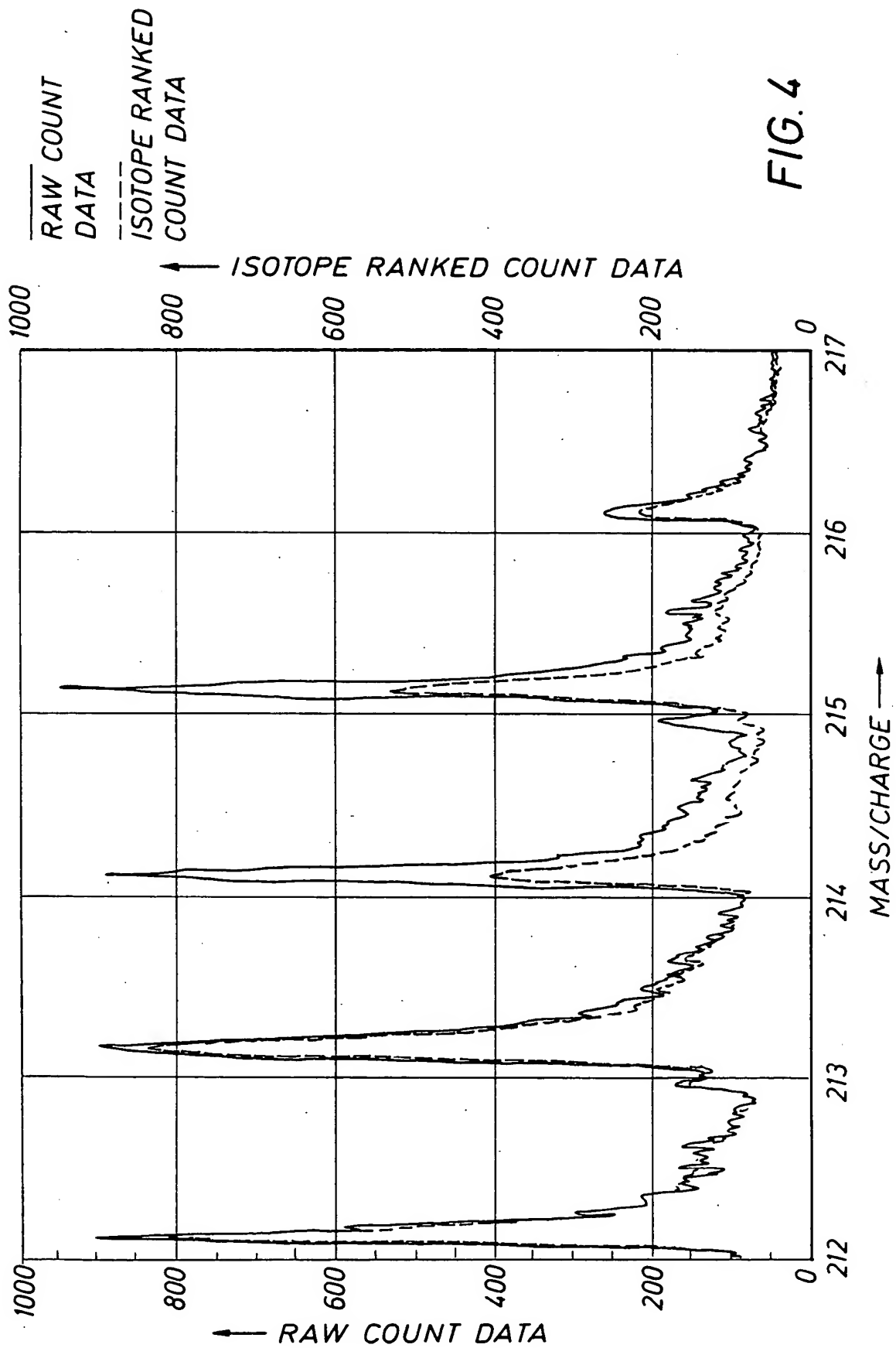


FIG. 4

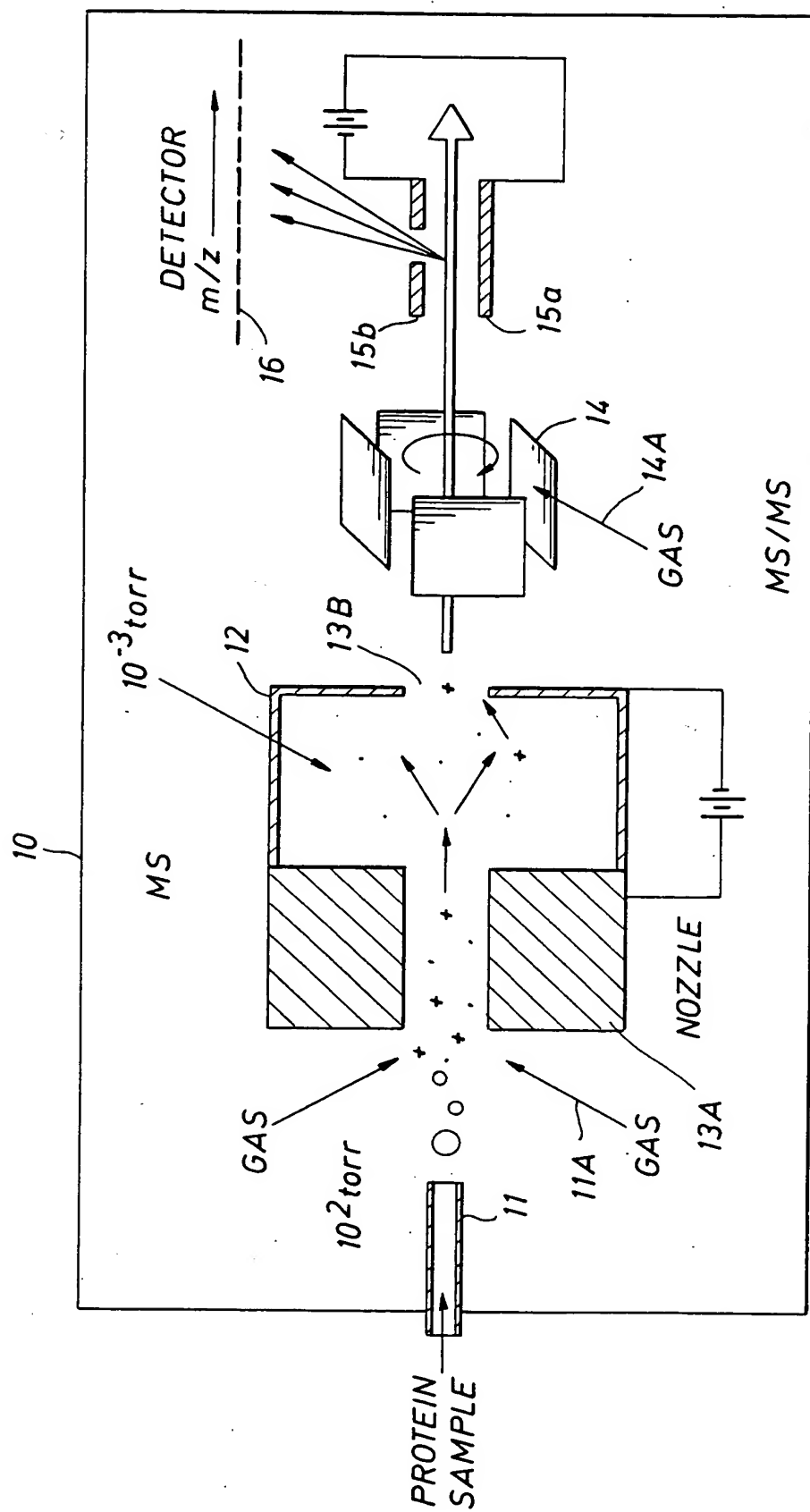


FIG. 5

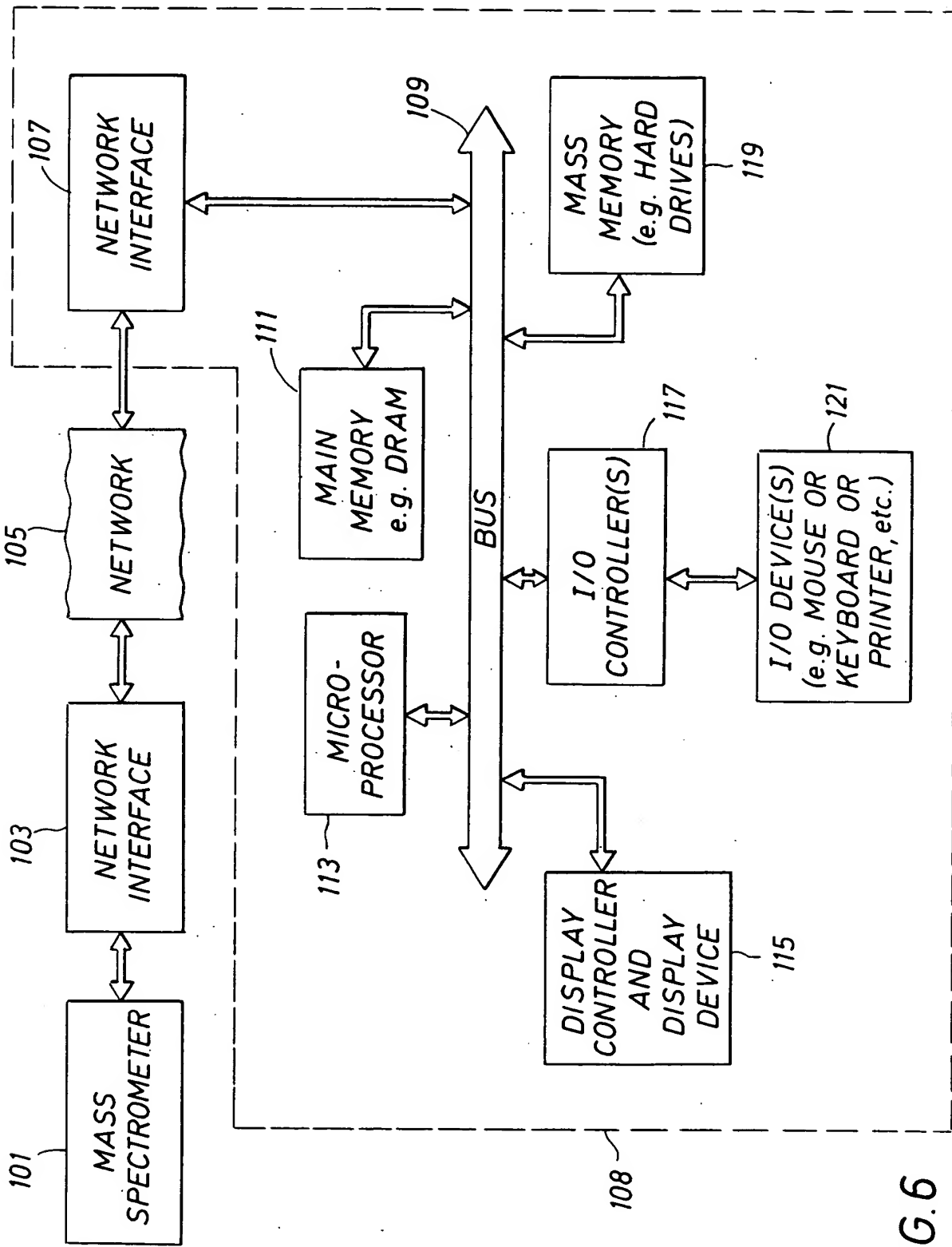


FIG. 6

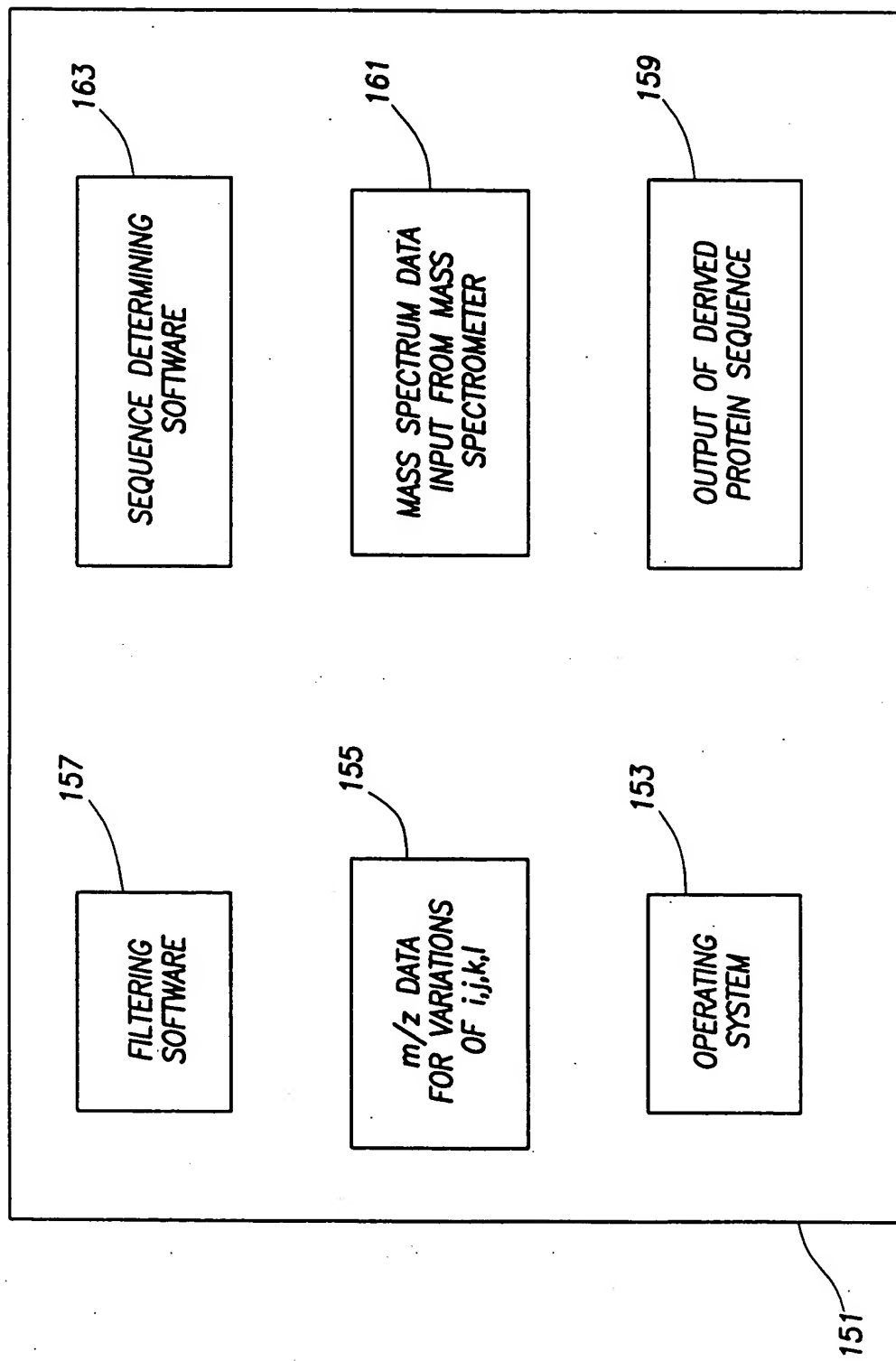
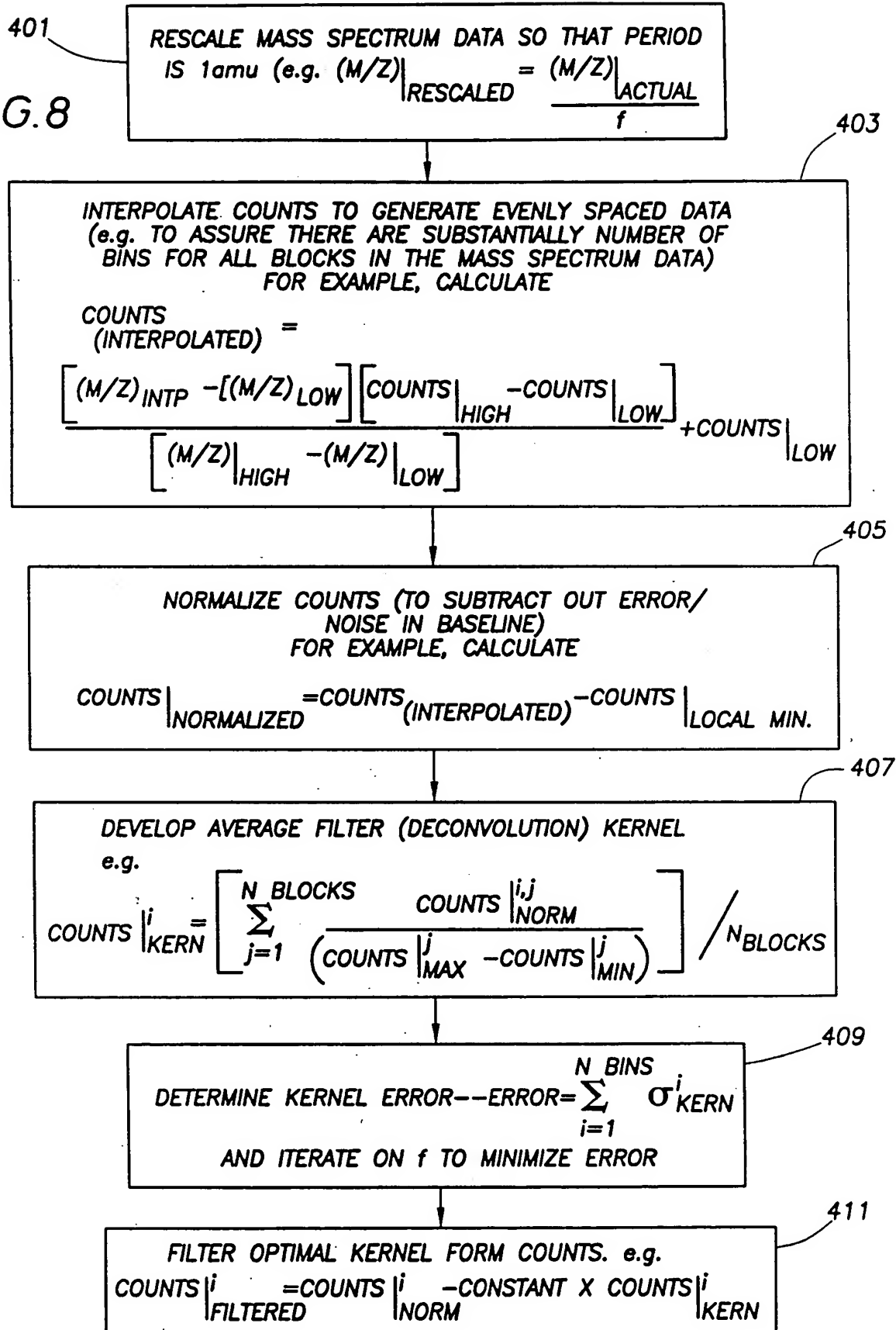
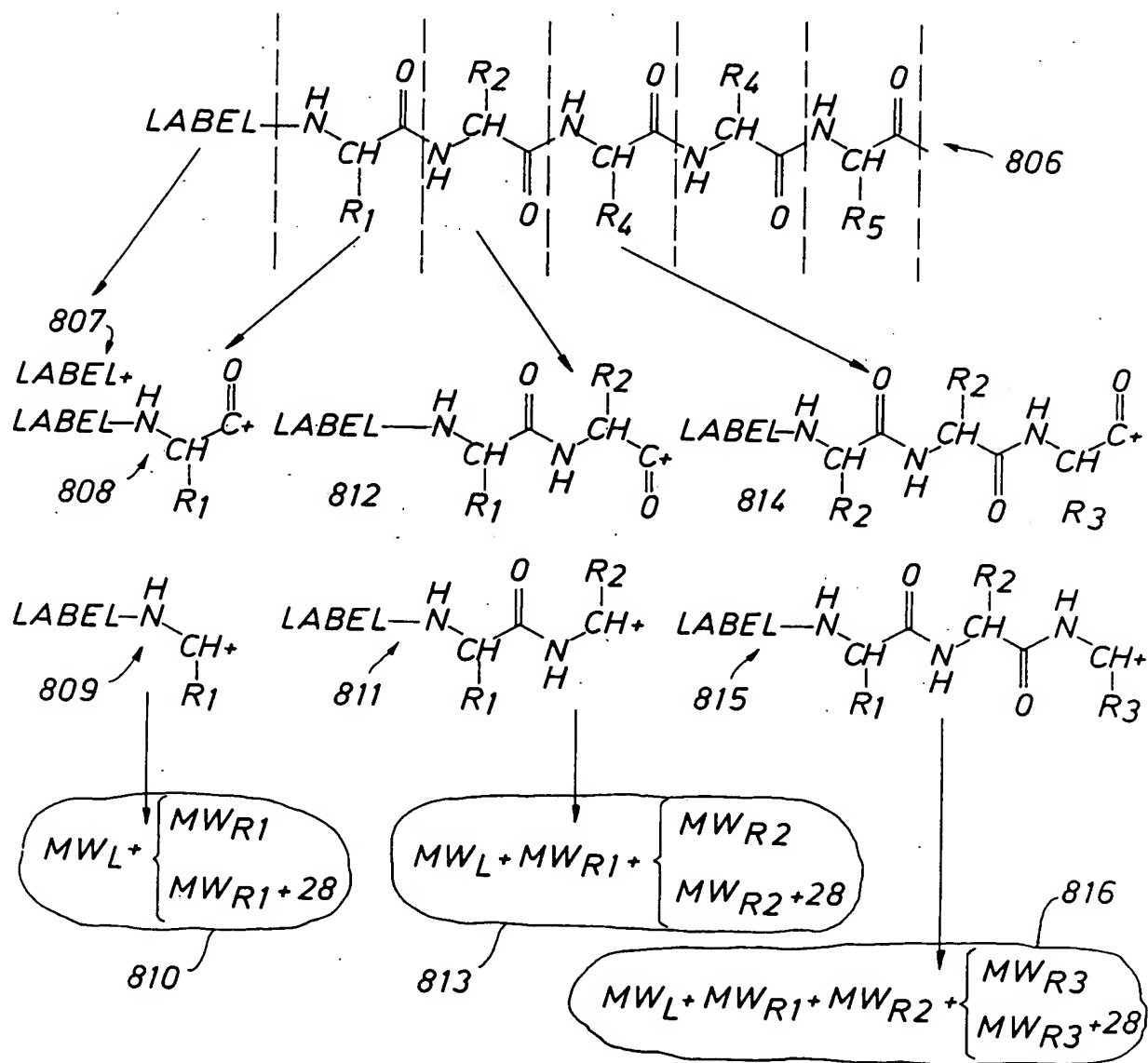
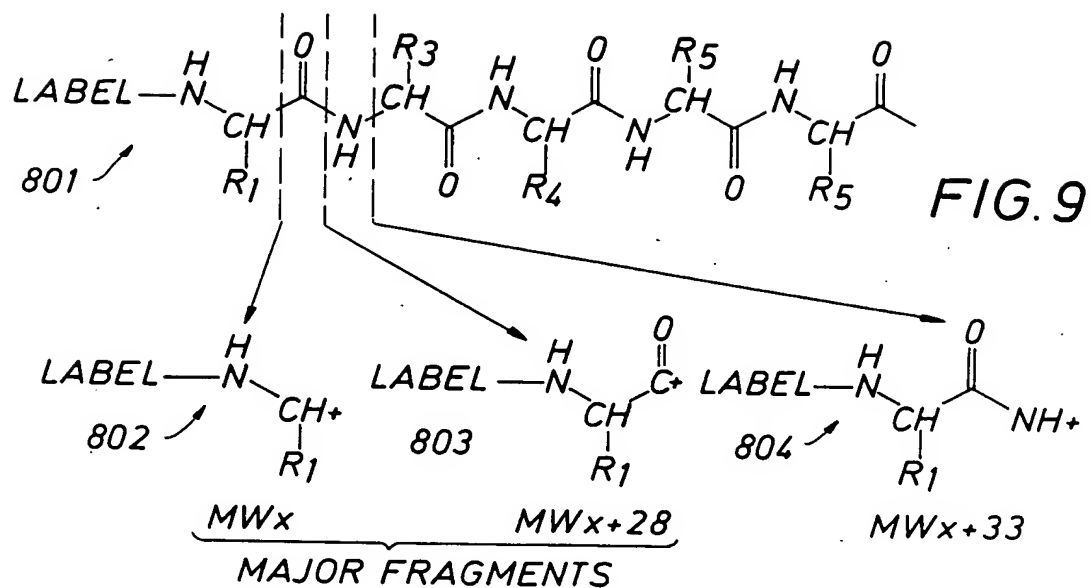


FIG. 7

FIG. 8



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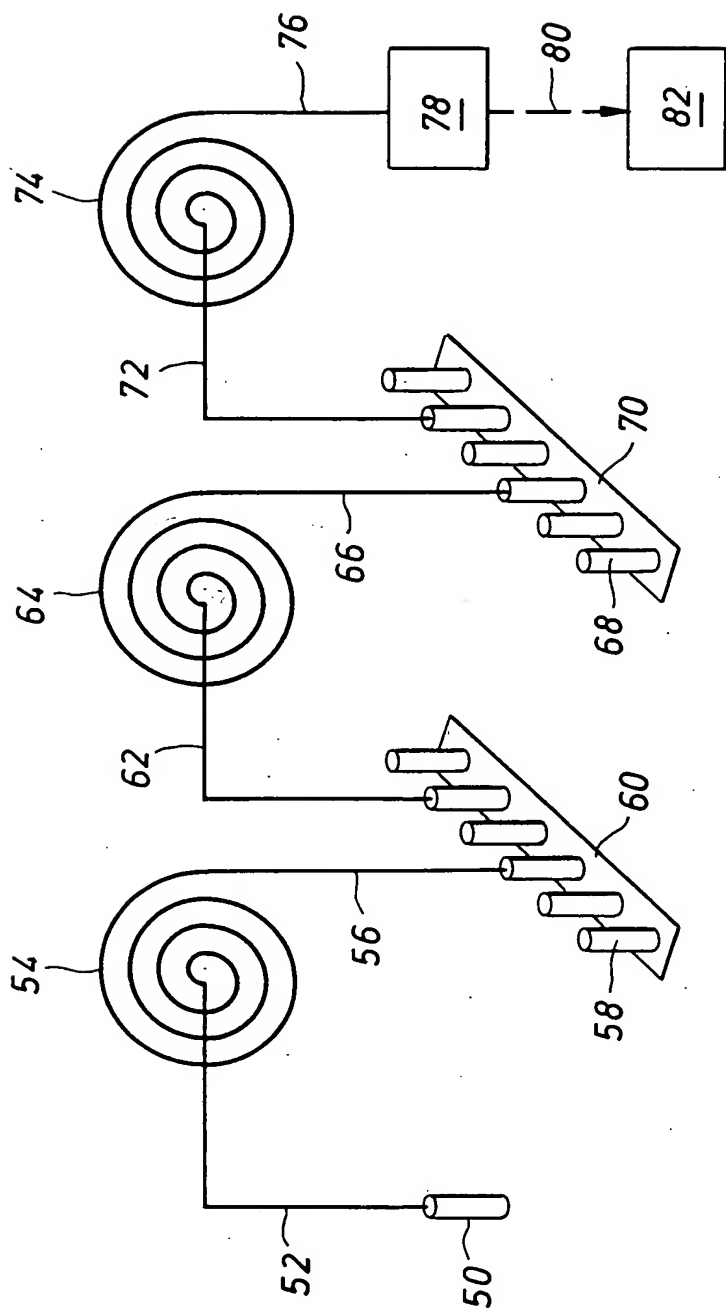
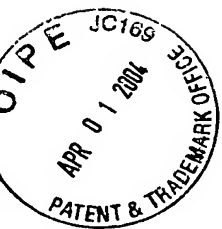


FIG.10

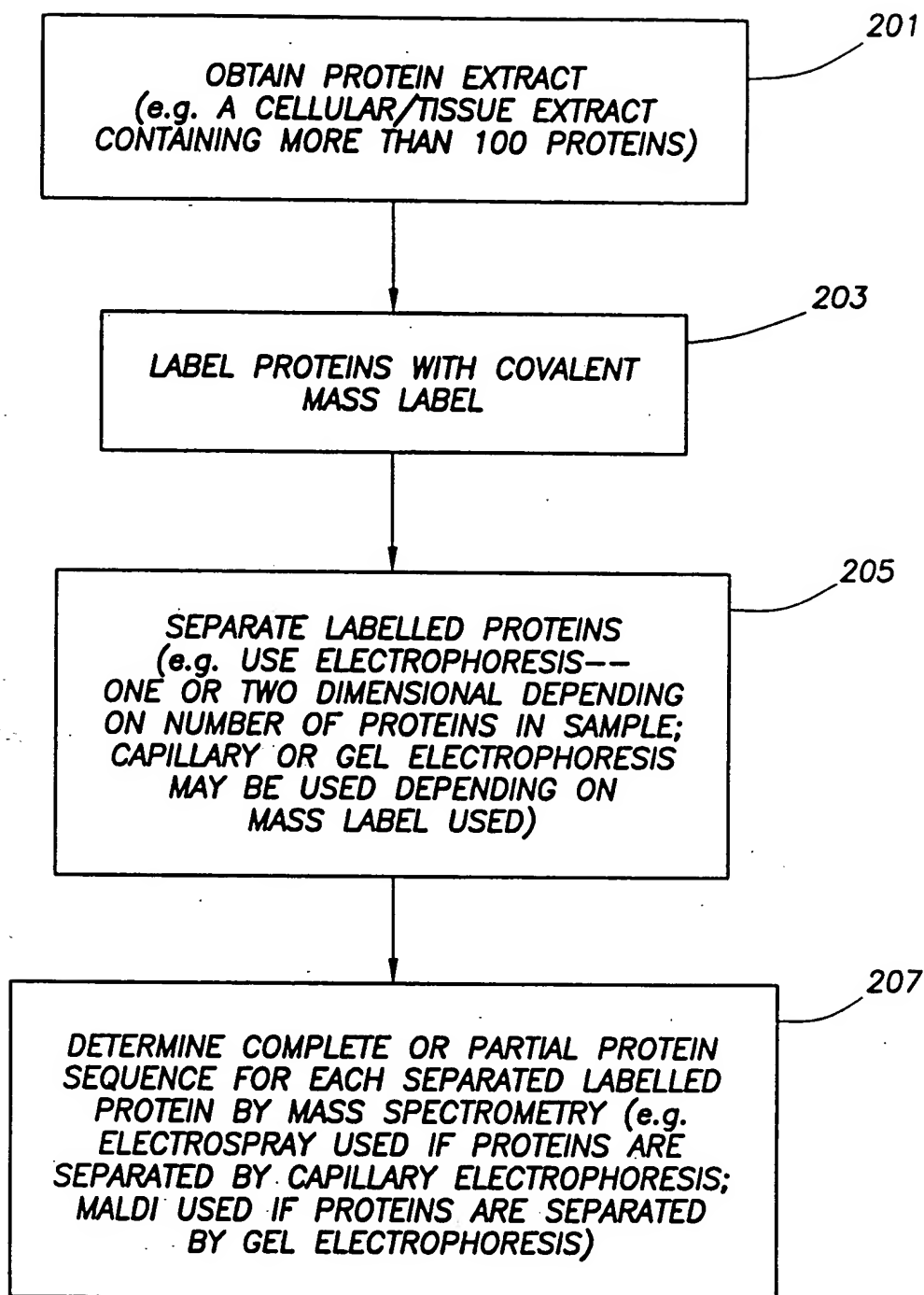
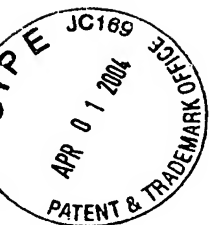


FIG.11

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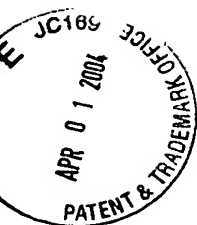
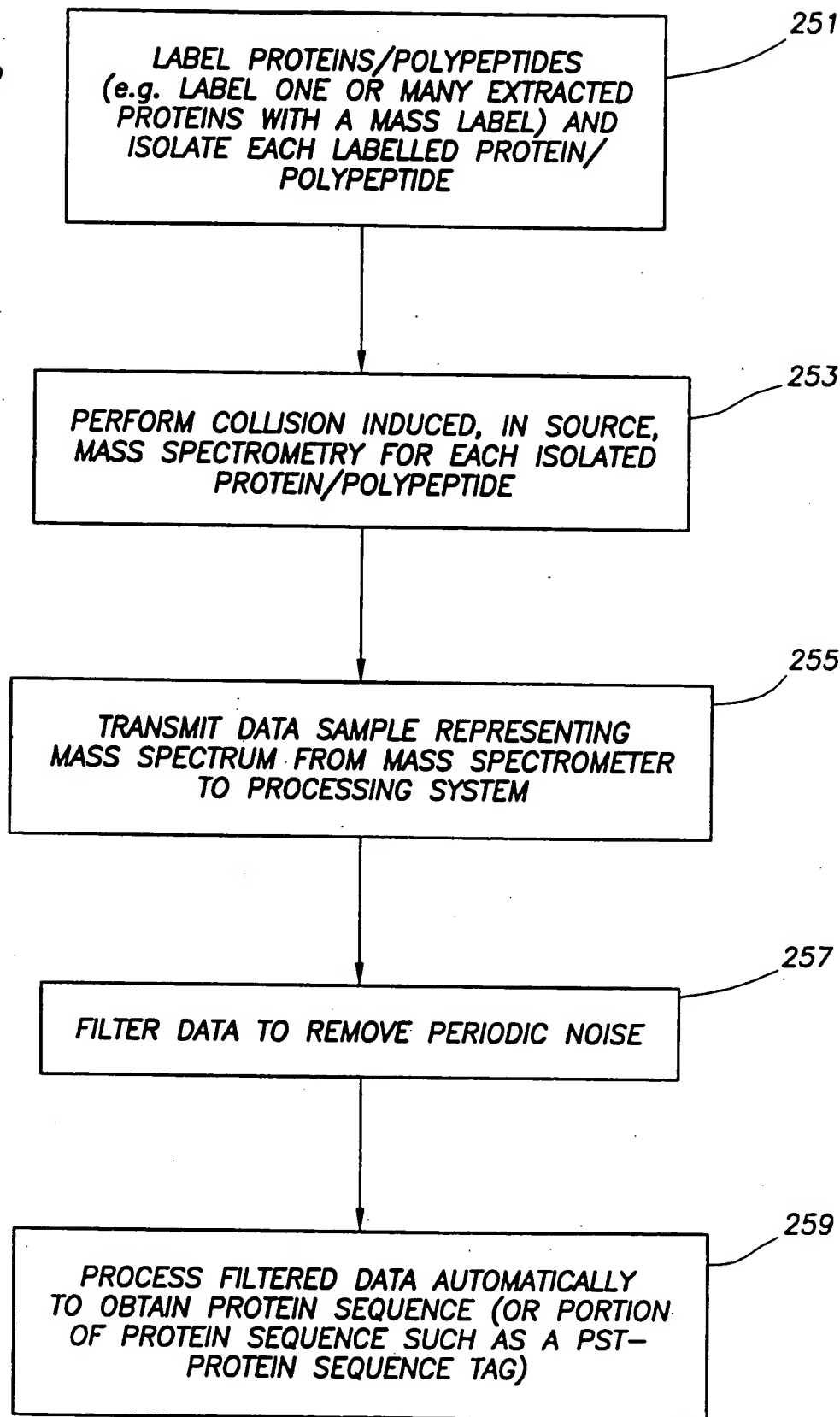


FIG.12



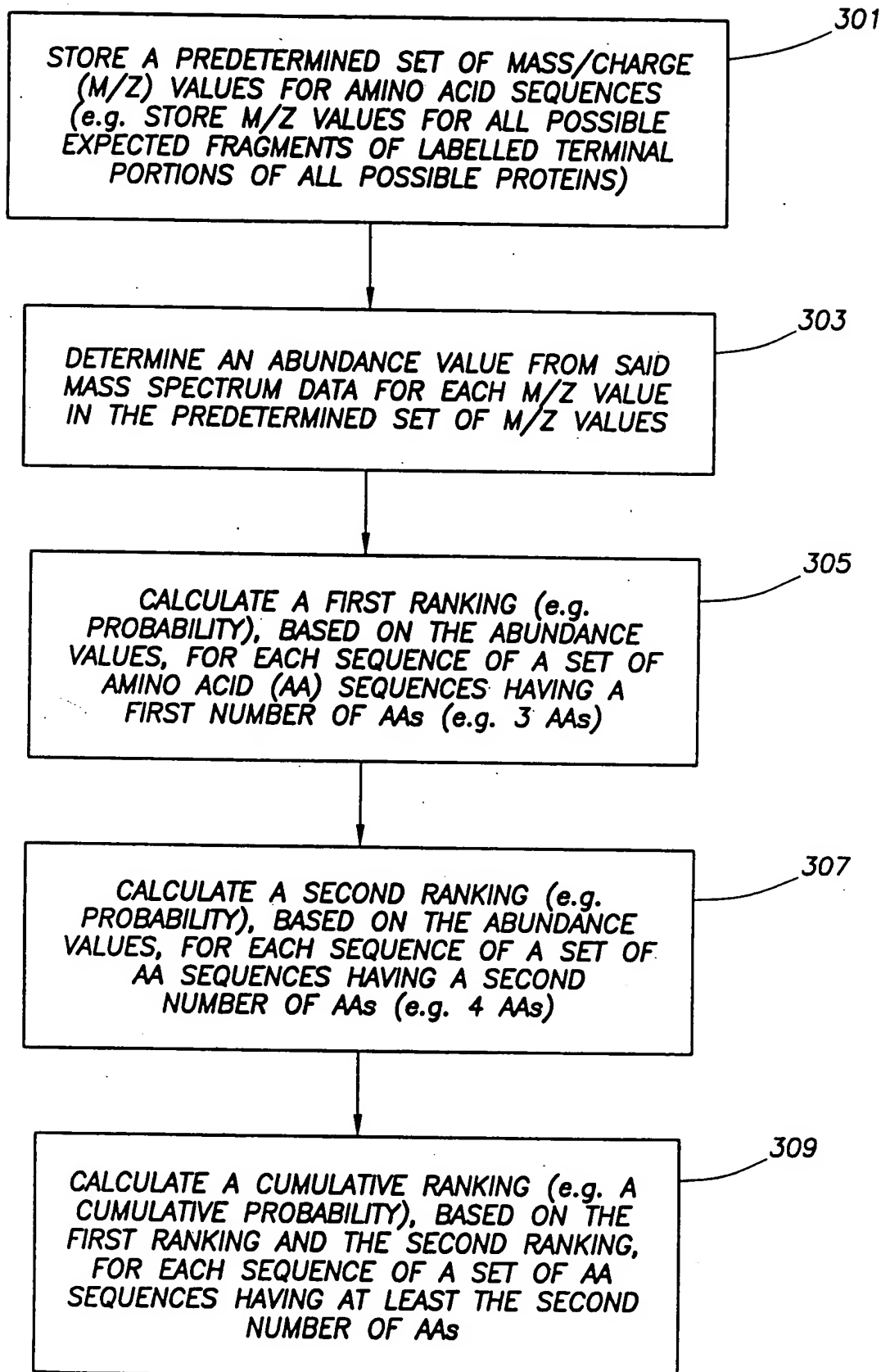
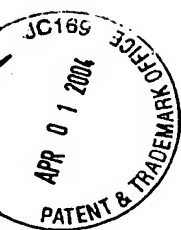


FIG. 13

FIG. 14A

FOR EACH POSSIBLE EXPECTED FRAGMENT OF A TERMINALLY LABELLED SEQUENCE OF AAs, PERFORM LOOKUP IN MASS SPECTRUM DATA FOR ABUNDANCE VALUE AT M/Z VALUE OF POSSIBLE EXPECTED FRAGMENT (e.g. $C_{i,j,k,l} = \text{LOOKUP} [(M/Z)_{i,j,k,l}]$)

DETERMINE MASTER COUNT, FOR EACH PARTICULAR POSSIBLE SEQUENCE, OVER ALL POSSIBLE ION TYPES AND CHARGE STATES FOR PARTICULAR SEQUENCE

e.g.

$$C_{i,j}^M = \sum_{l=\text{MIN CHARGE STATES}}^{\text{MAX CHARGE STATES}} \left(\sum_{k=1}^{\text{MAX ION TYPES}} C_{i,j,k,l} \right)$$

WHERE

i =NUMBER OF AMINO ACIDS (AAs) IN SEQUENCE
 j =NUMBER OF POSSIBLE SEQUENCES (USUALLY, 19^i)
 l =NUMBER OF ION TYPES FOR EACH RESIDUE (e.g. ION TYPES a,b, AND POSSIBLY c AT N TERMINUS AND ION TYPES x,y, AND POSSIBLY z AT C TERMINUS)
 k =NUMBER OF CHARGE STATES FOR EACH ION TYPE

FOR EACH MASTER COUNT ($C_{i,j}^M$) FOR A PARTICULAR POSSIBLE SEQUENCE AT A GIVEN SEQUENCE LENGTH, COMPARE THE MASTER COUNT TO ALL OTHER MASTER COUNTS FOR ALL OTHER POSSIBLE SEQUENCES FOR THE GIVEN SEQUENCE LENGTH TO PRODUCE A RANKING OF MASTER COUNTS OF ALL POSSIBLE SEQUENCES AT THE GIVEN LENGTH OF AAs. FOR EXAMPLE, THE COMPARISON MAY BE A RANKING OF PROBABILITIES WHERE EACH PROBABILITY IS A PROBABILITY OF A PARTICULAR SEQUENCE AT THE GIVEN SEQUENCE LENGTH RELATIVE TO ALL OTHER POSSIBLE SEQUENCES AT THE SAME LENGTH

TO FIG. 14B

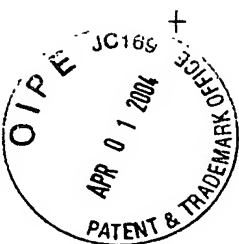


FIG. 14B

FROM FIG. 14A

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IN ONE EXAMPLE, DETERMINE P_i (A FIRST RANKING) EACH PARTICULAR POSSIBLE SEQUENCE j AT A GIVEN AA LENGTH i :

$$P_i = \text{NORMAL DISTRIBUTION} \left[\frac{c_{i,j}^M - \bar{c}_i}{\sigma_i} \right]$$

WHERE:

$$\bar{c}_i = \left(\sum_{j=1}^{19^i} c_{i,j}^M \right) / 19^i$$

AND

$$\sigma_i = \sqrt{\frac{\sum_{j=1}^{19^i} (c_{i,j}^M)^2 - \frac{(\bar{c}_i)^2}{19^i}}{(19^i - 1)}}$$

DETERMINE CUMULATIVE RANKING FOR A GIVEN SEQUENCE OVER DIFFERENT SEQUENCE LENGTHS --e.g. CALCULATE

$$R_{j,n} = \prod_{i=1}^n P_i \quad \text{OR} \quad = \sum_{i=1}^n P_i$$

e.g. $P[C_{2,j=A-A}^M] + P[C_{3,j=A-A-X}^M] = \text{CUMULATIVE RANKING}$

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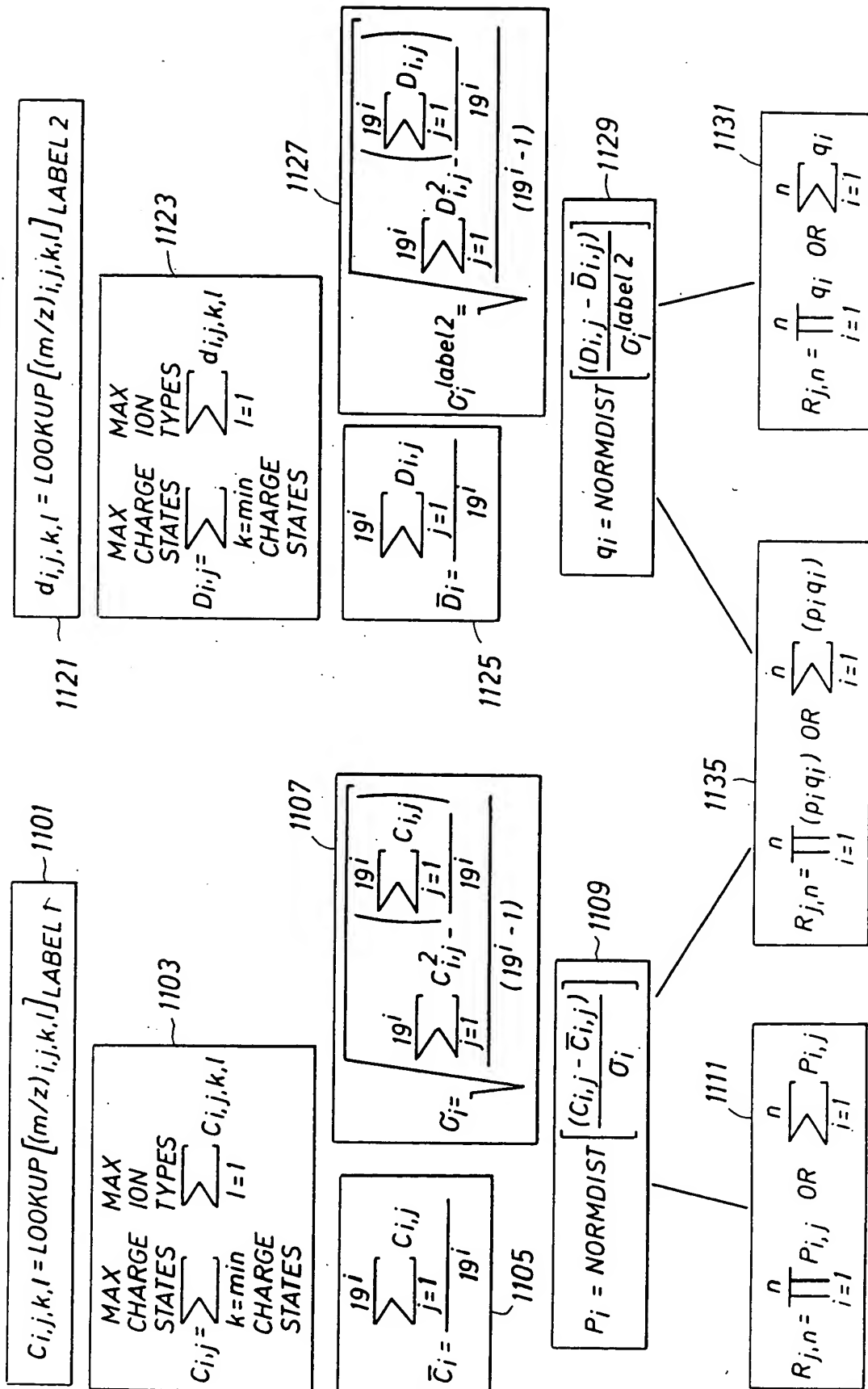
SELECT SEQUENCE WITH HIGHEST CUMULATIVE RANKING

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FIG. 15

LABEL 1

LABEL 2



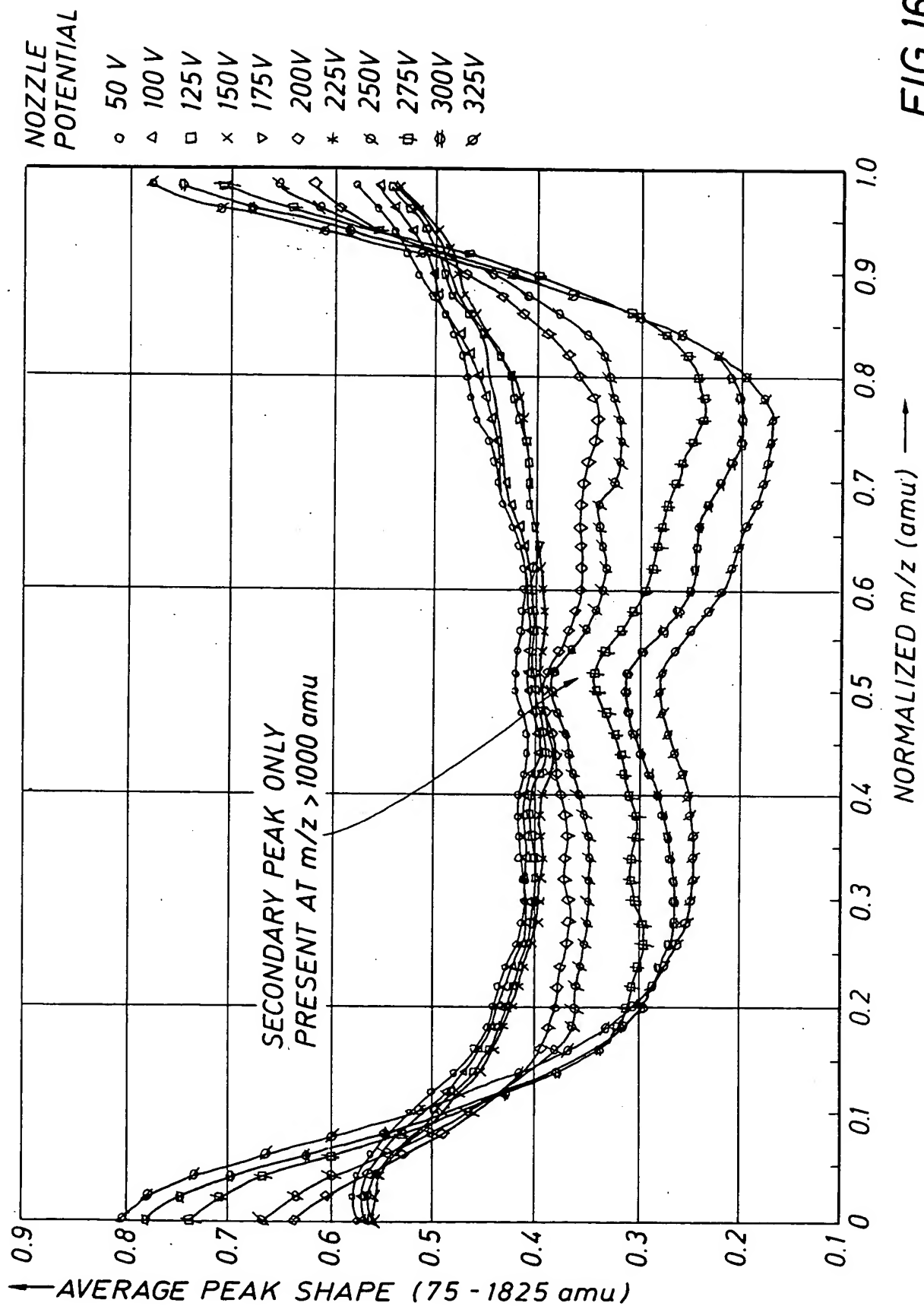


FIG.16

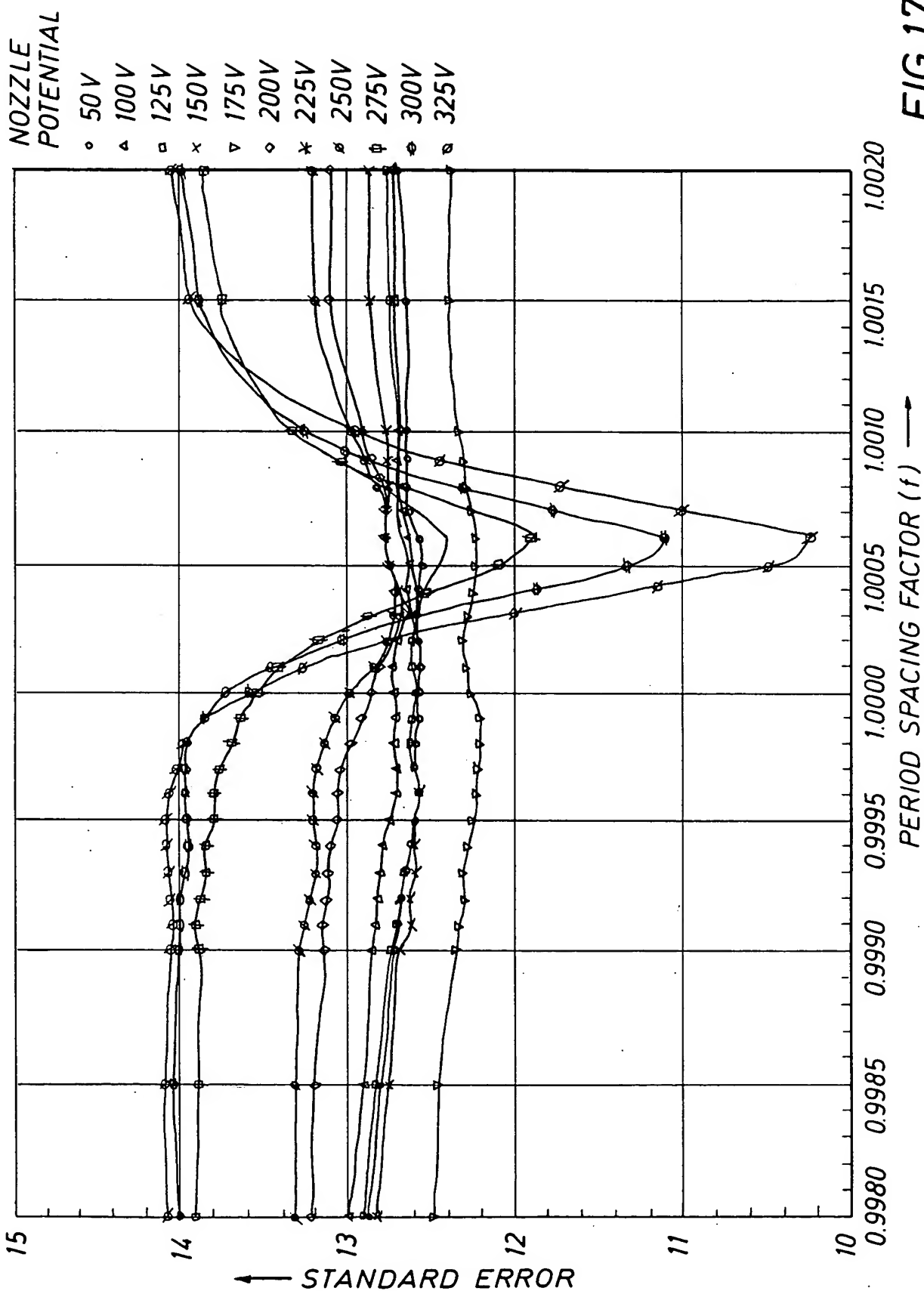


FIG.17

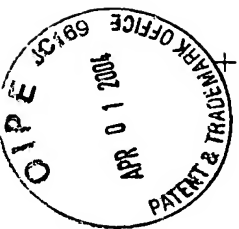
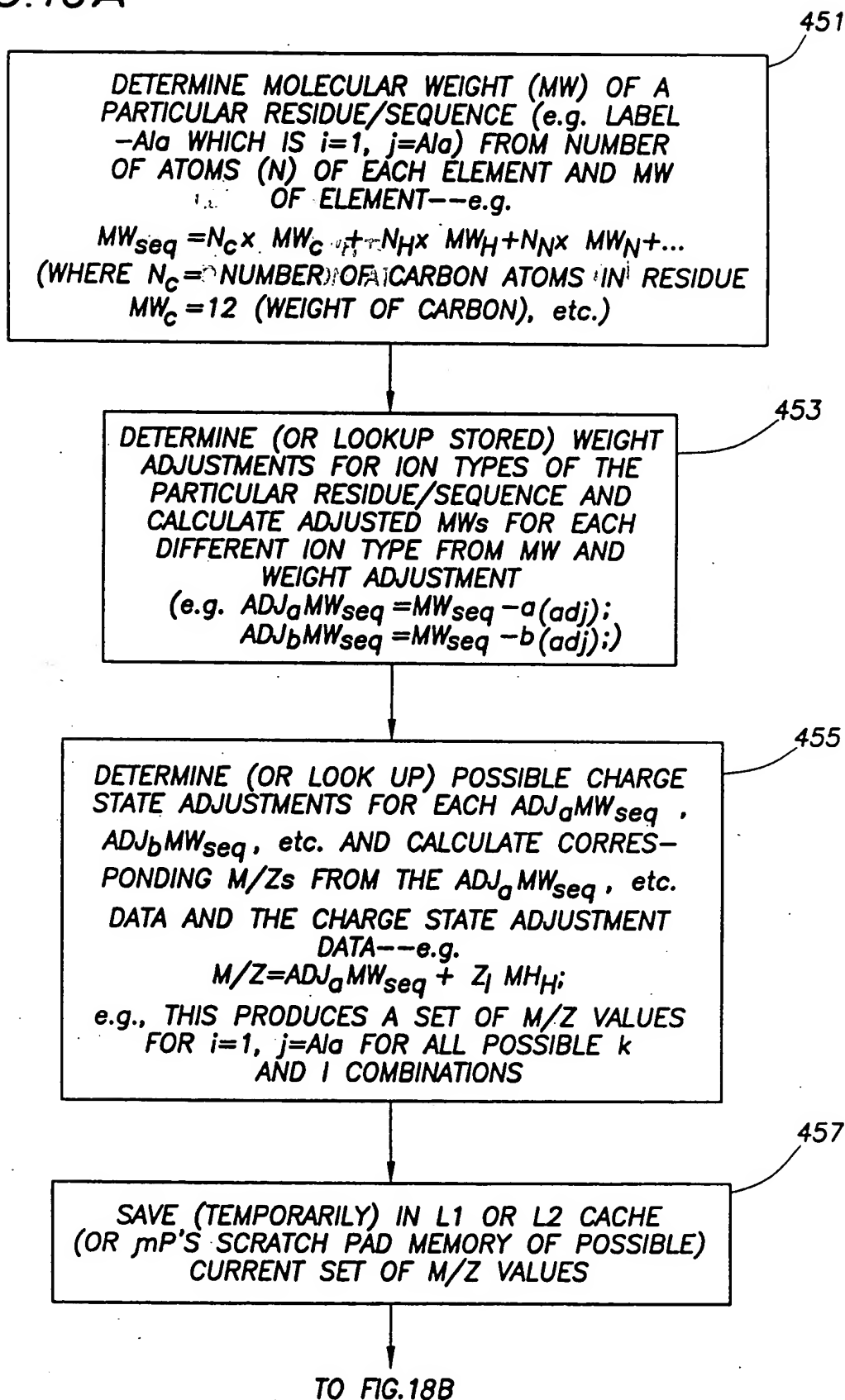


FIG. 18A



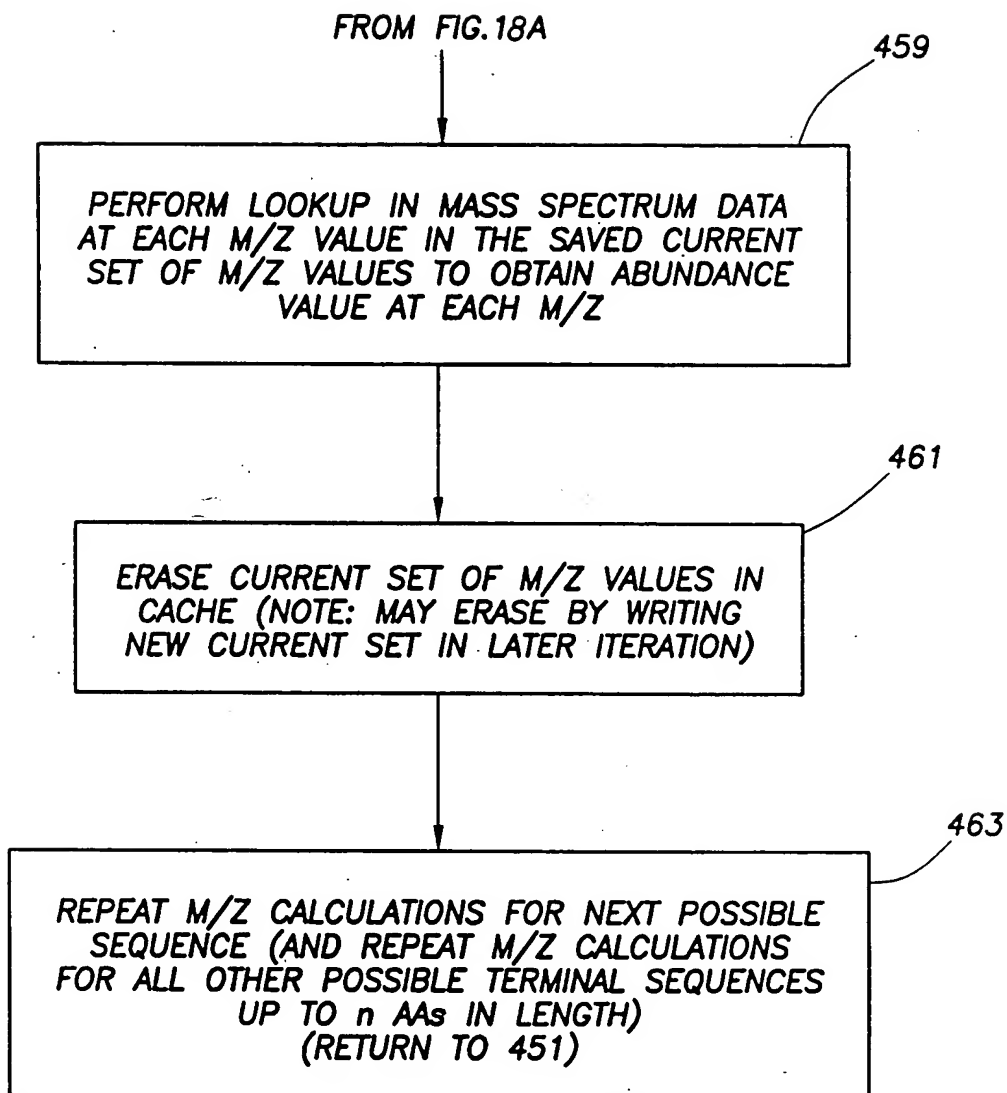
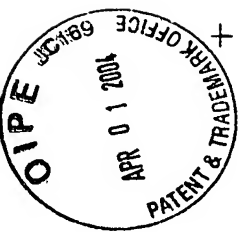


FIG.18B

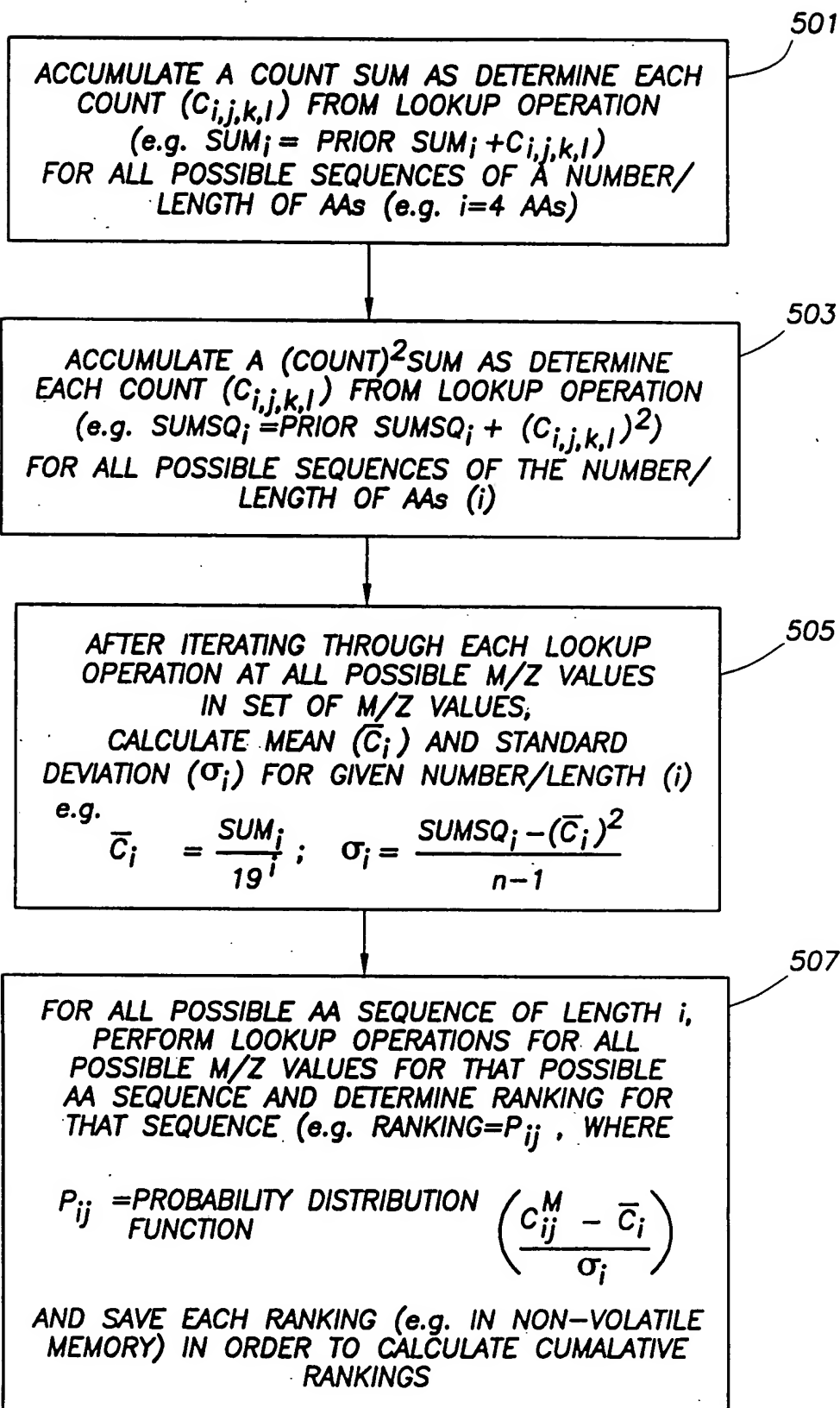
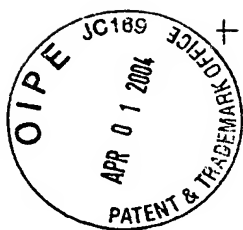


FIG. 19

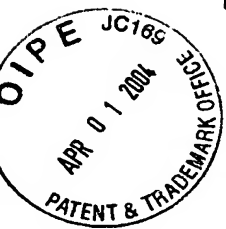


FIG. 20A

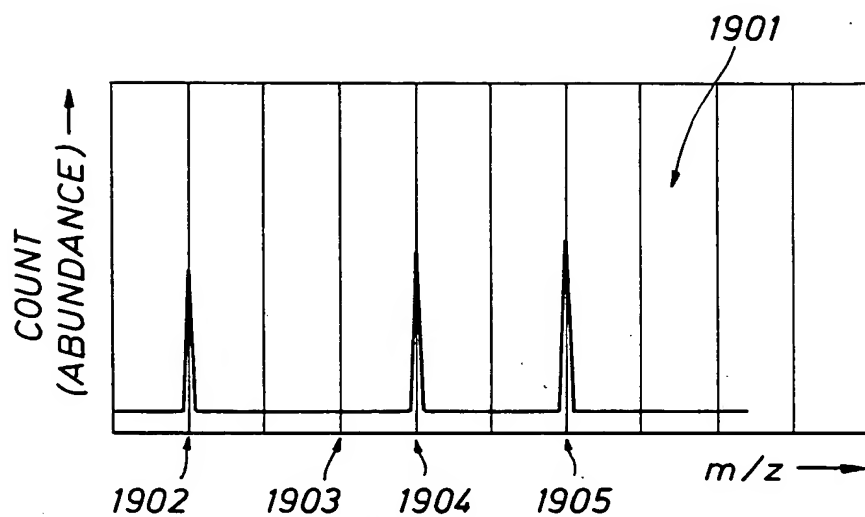
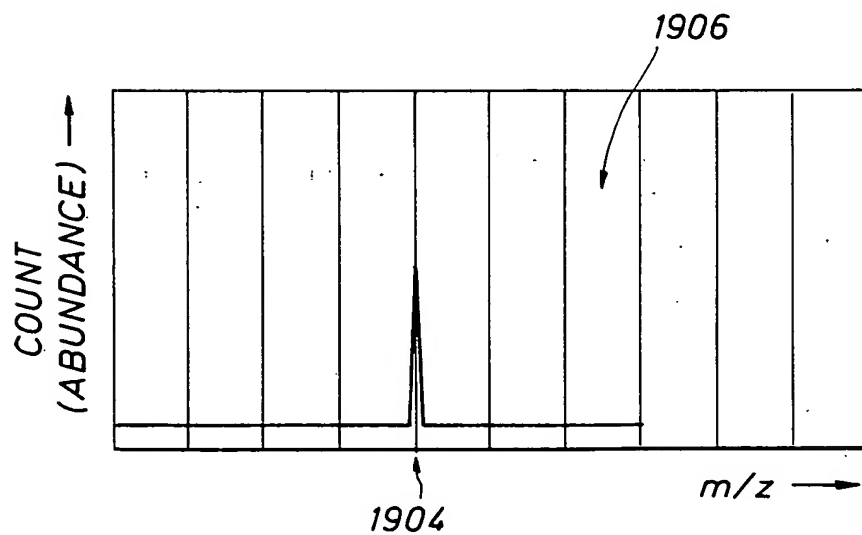


FIG. 20B



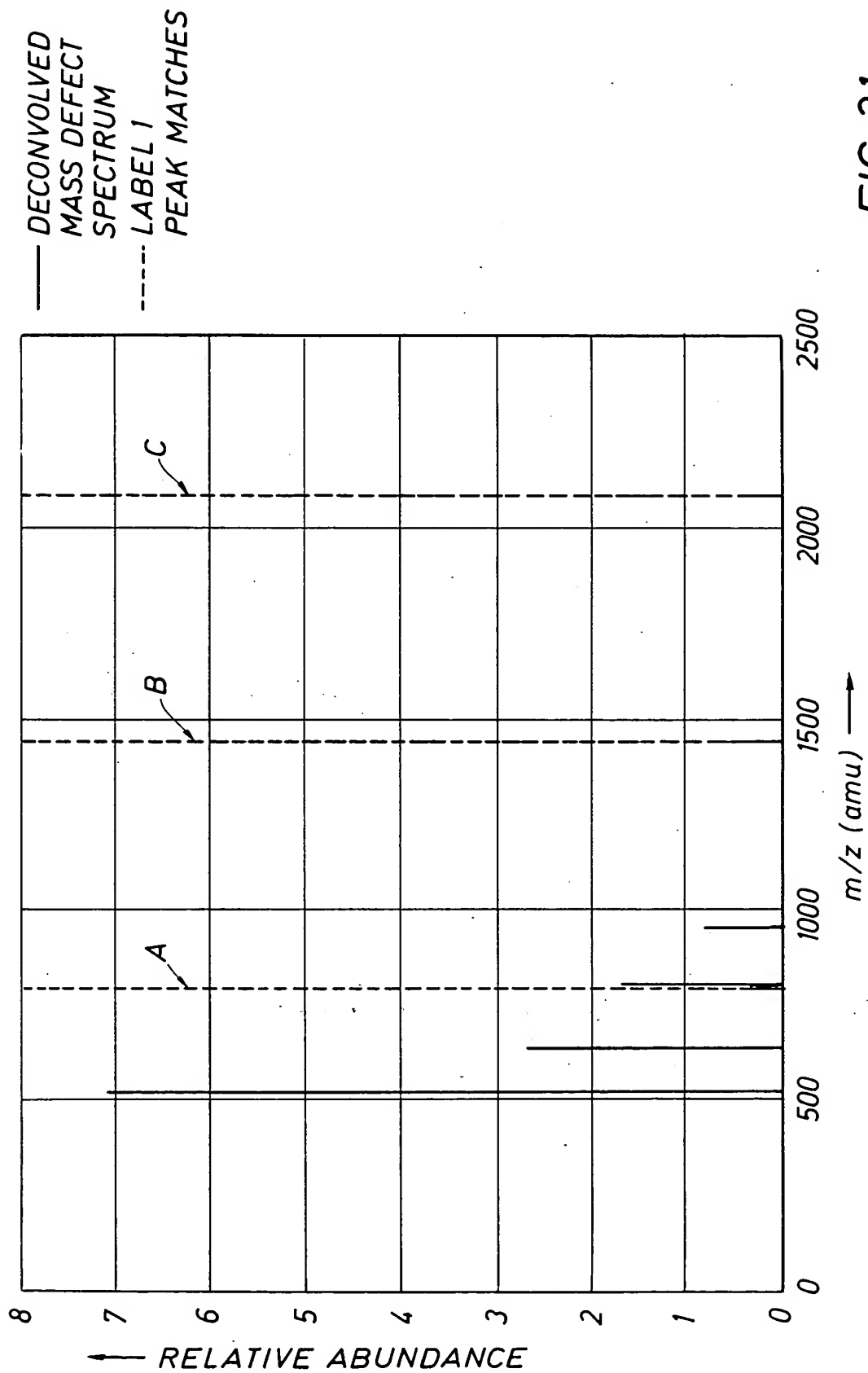
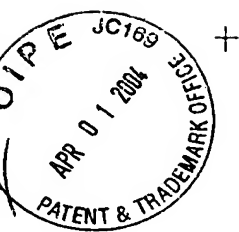


FIG. 21

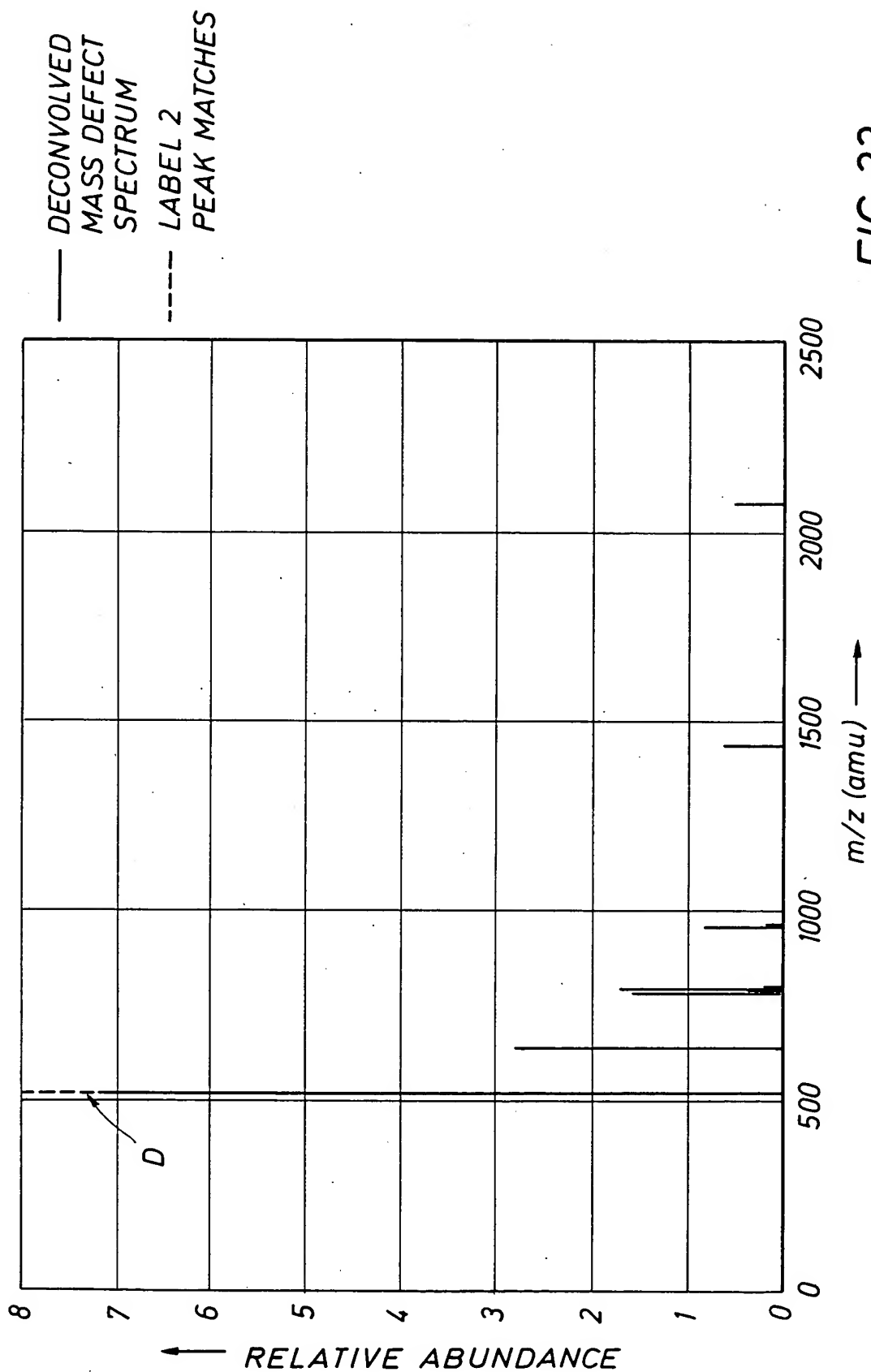
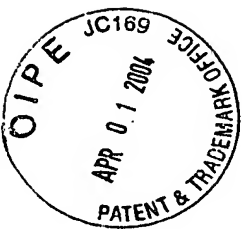


FIG. 22

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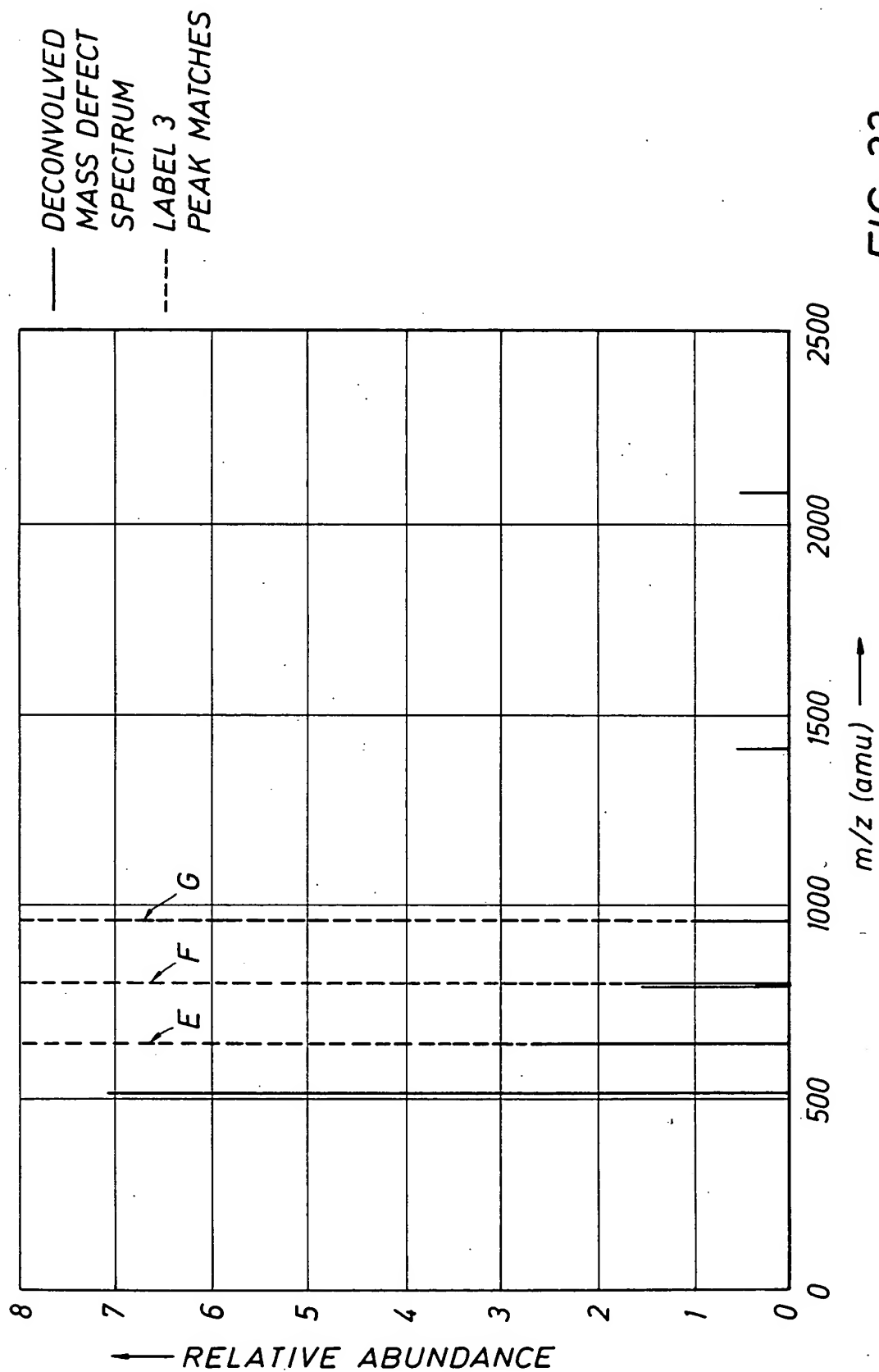
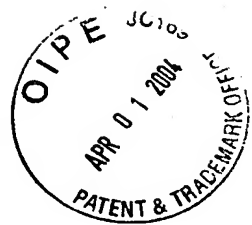


FIG. 23

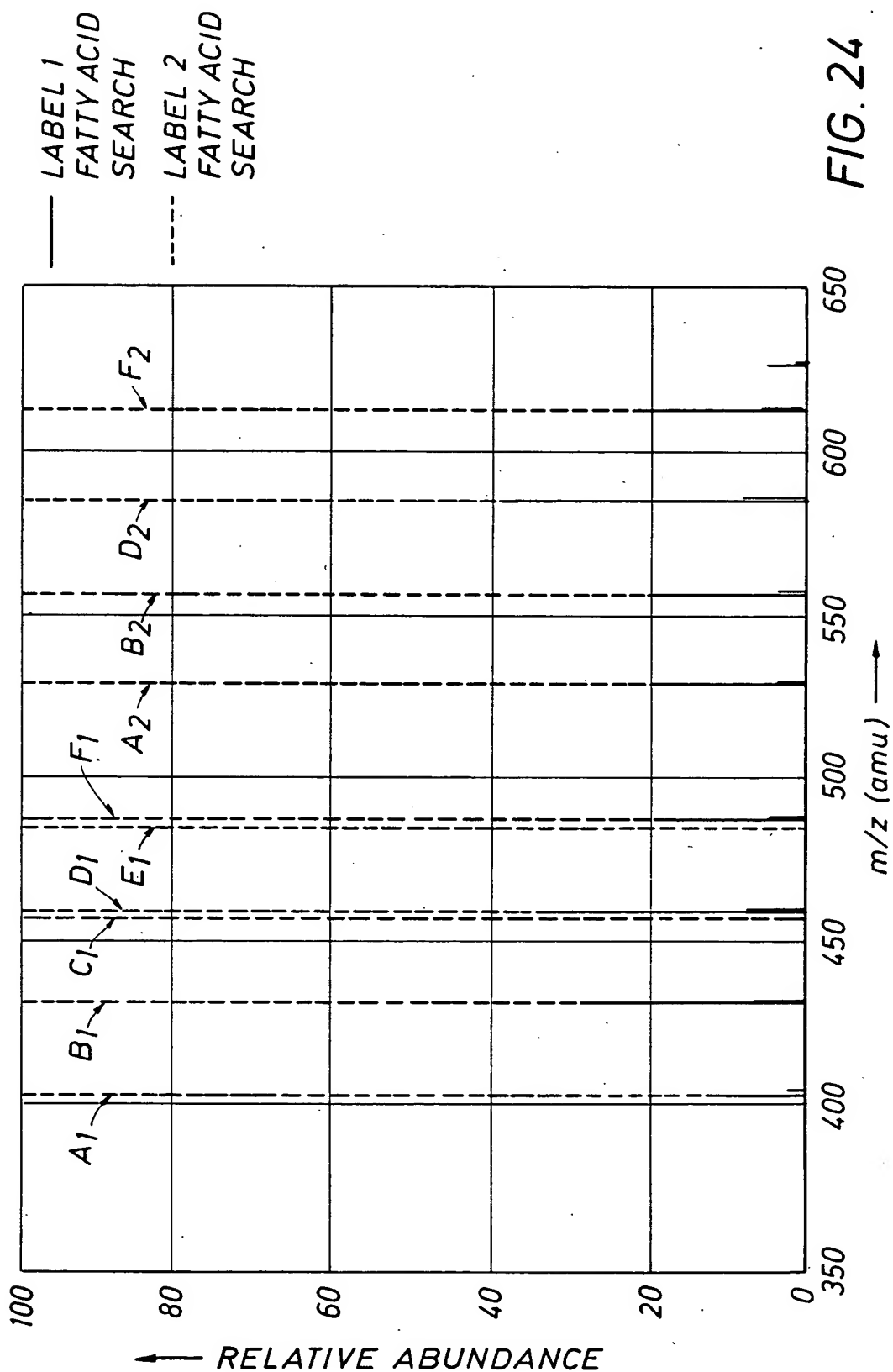
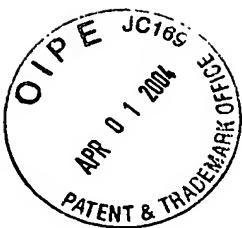


FIG. 24

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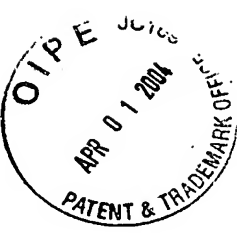


FIG. 25

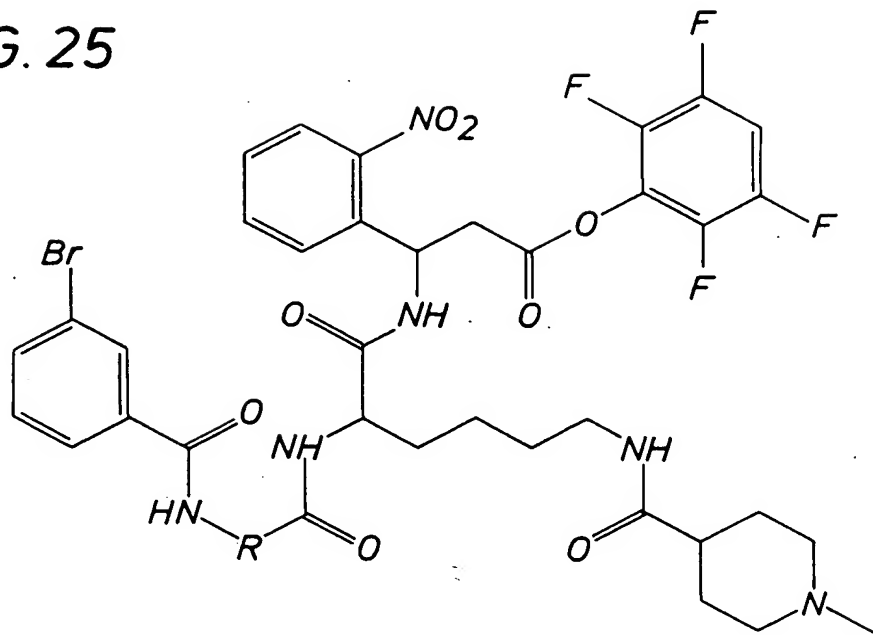
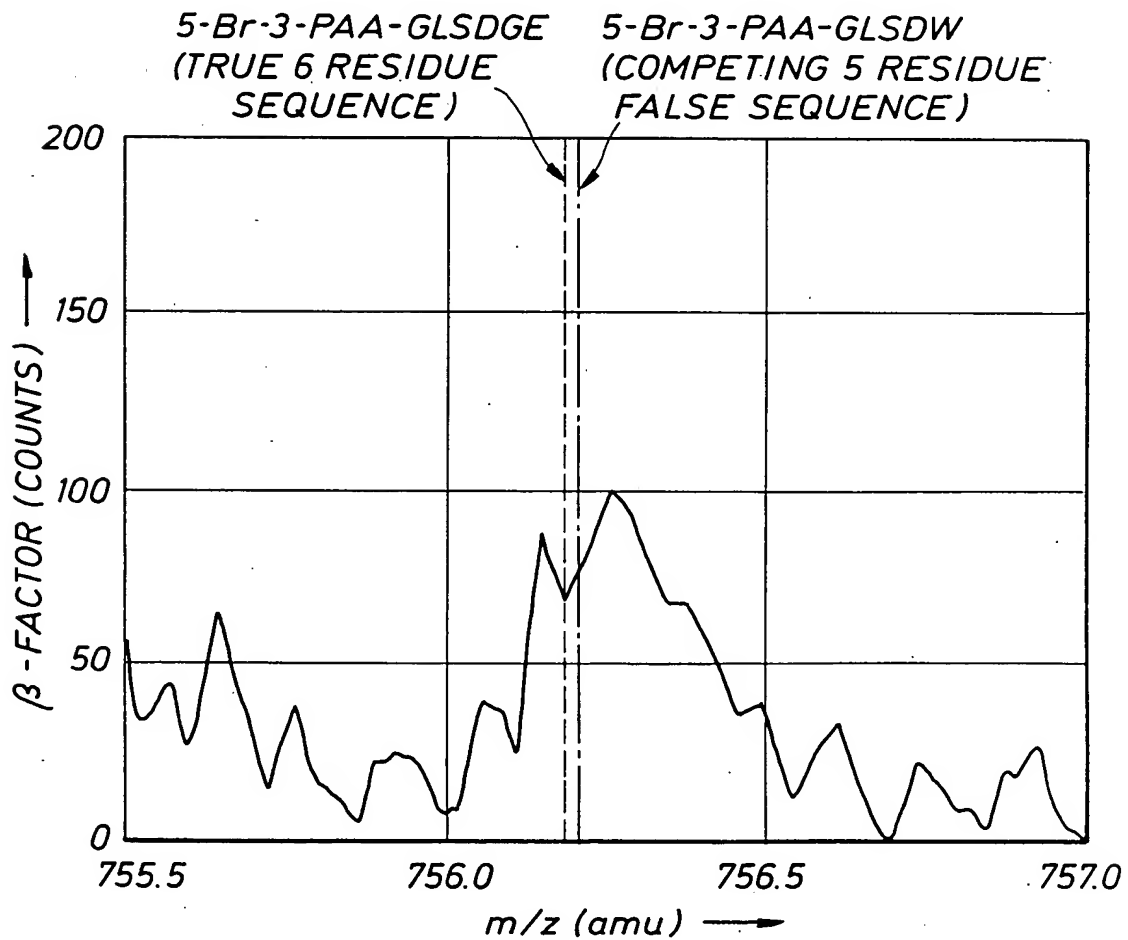


FIG. 33



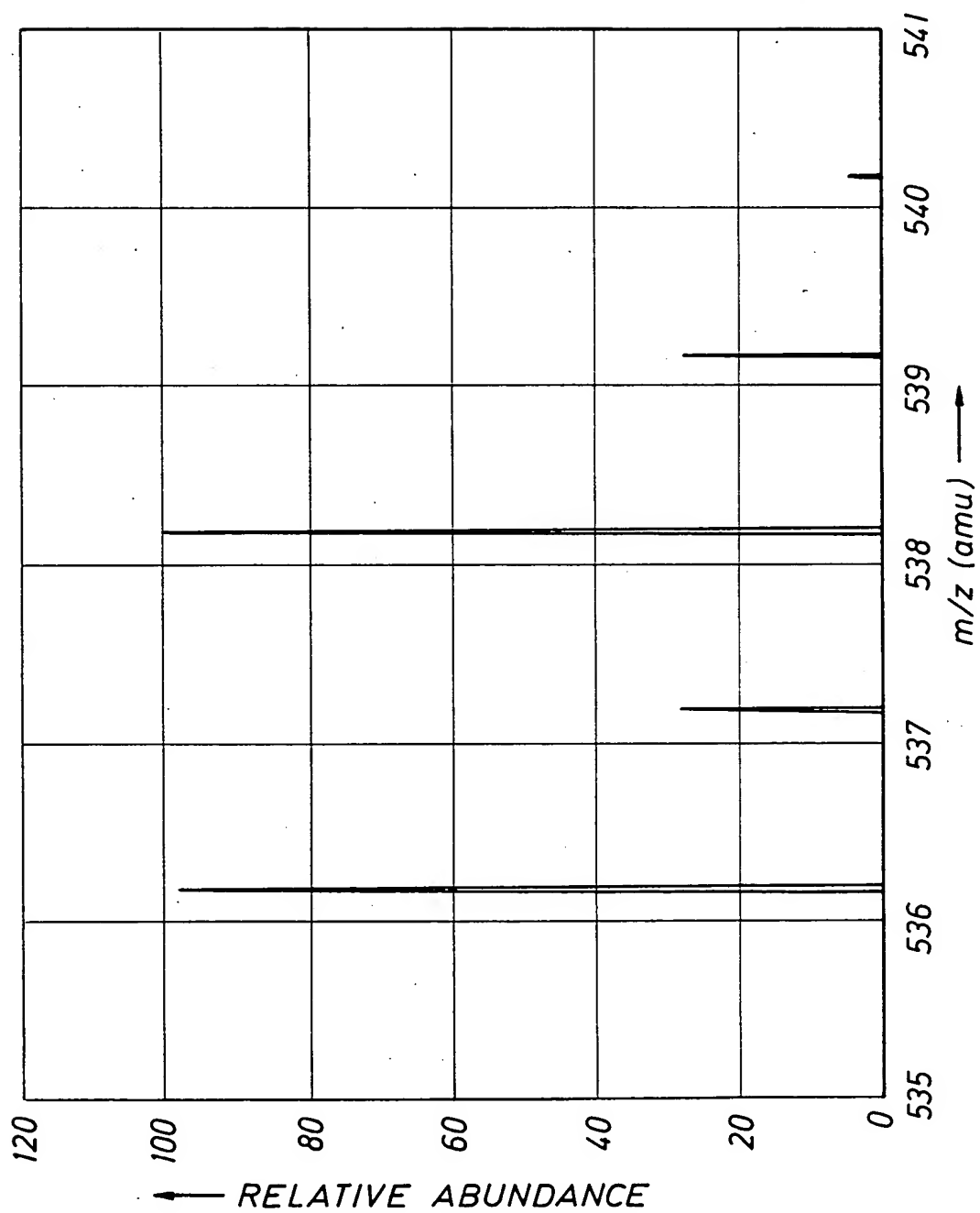
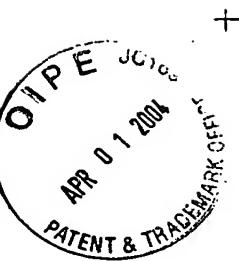


FIG. 26

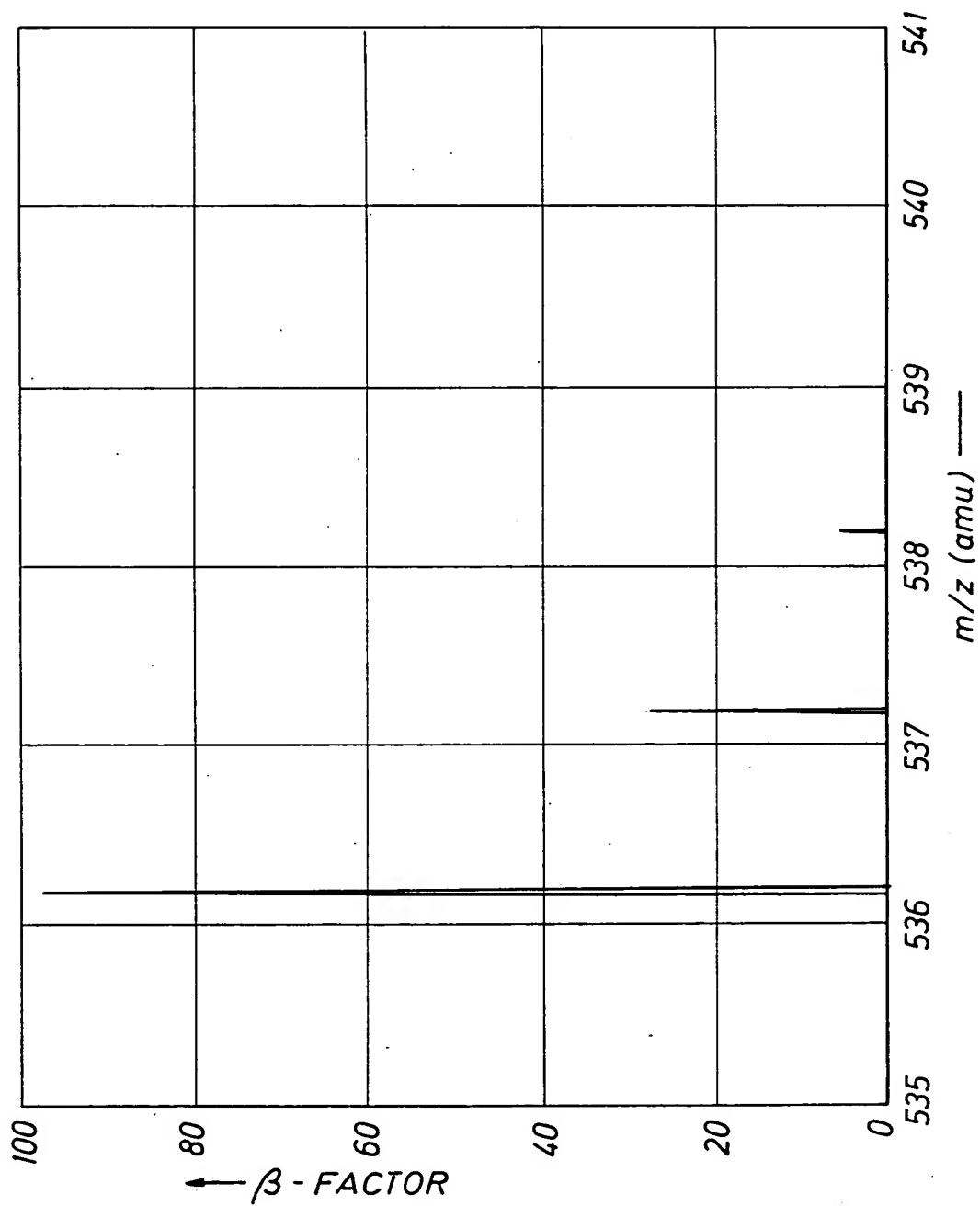
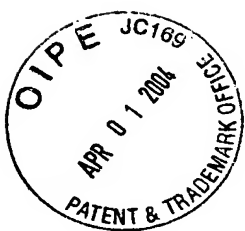


FIG. 27

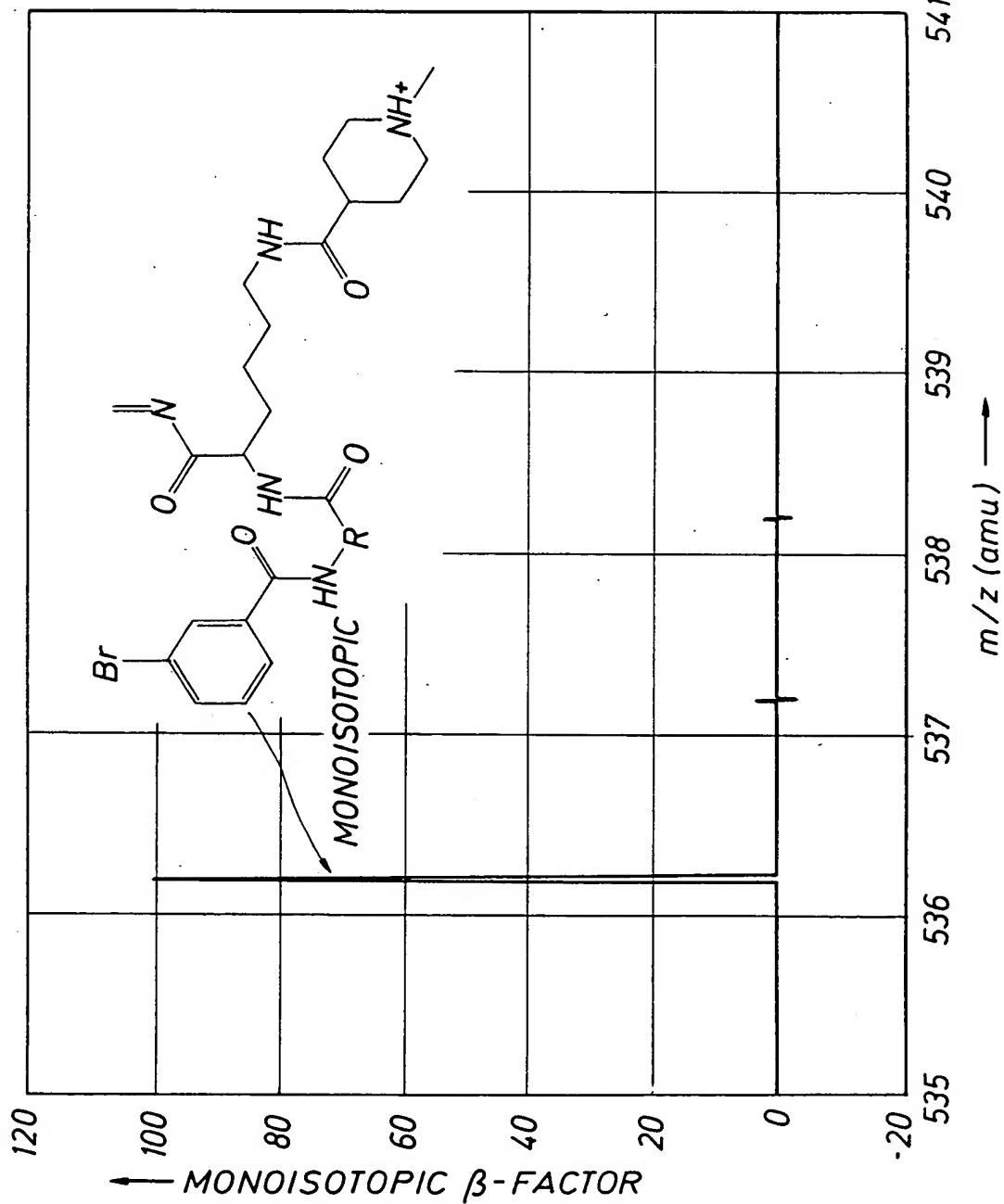
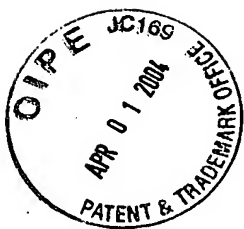


FIG. 28

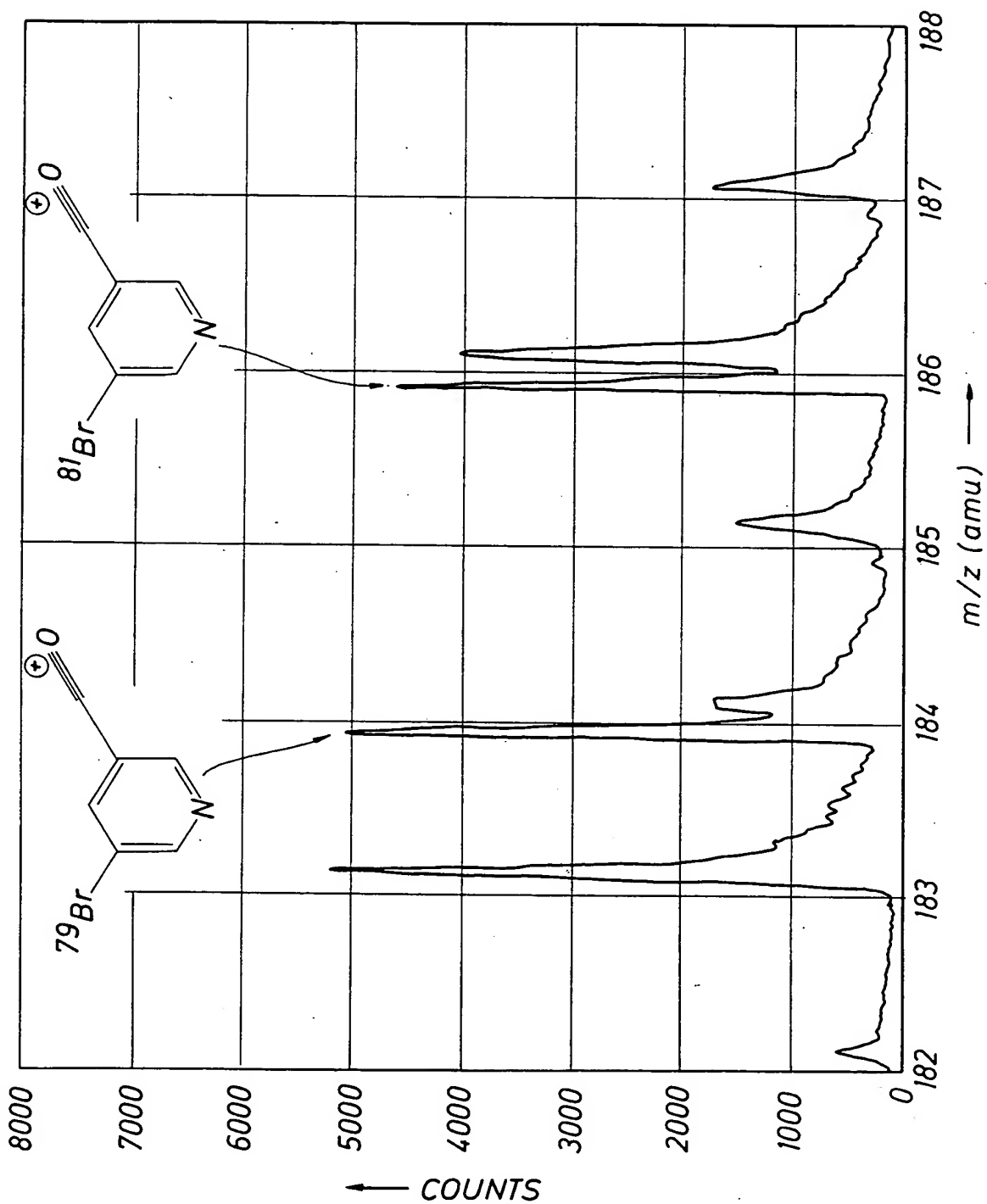
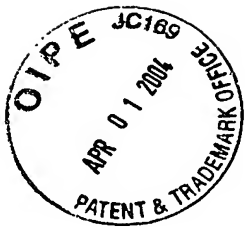


FIG. 29

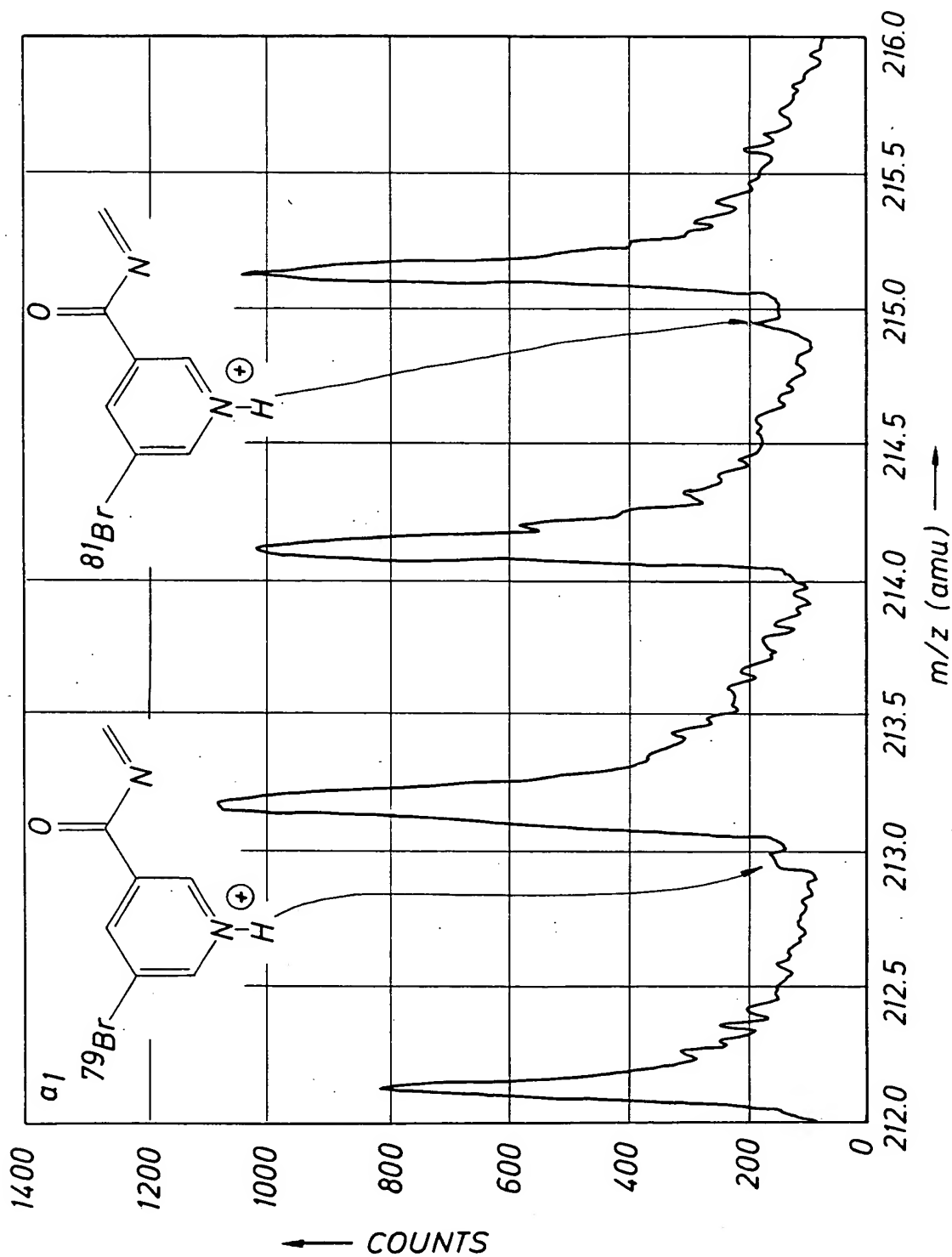
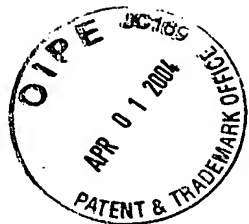
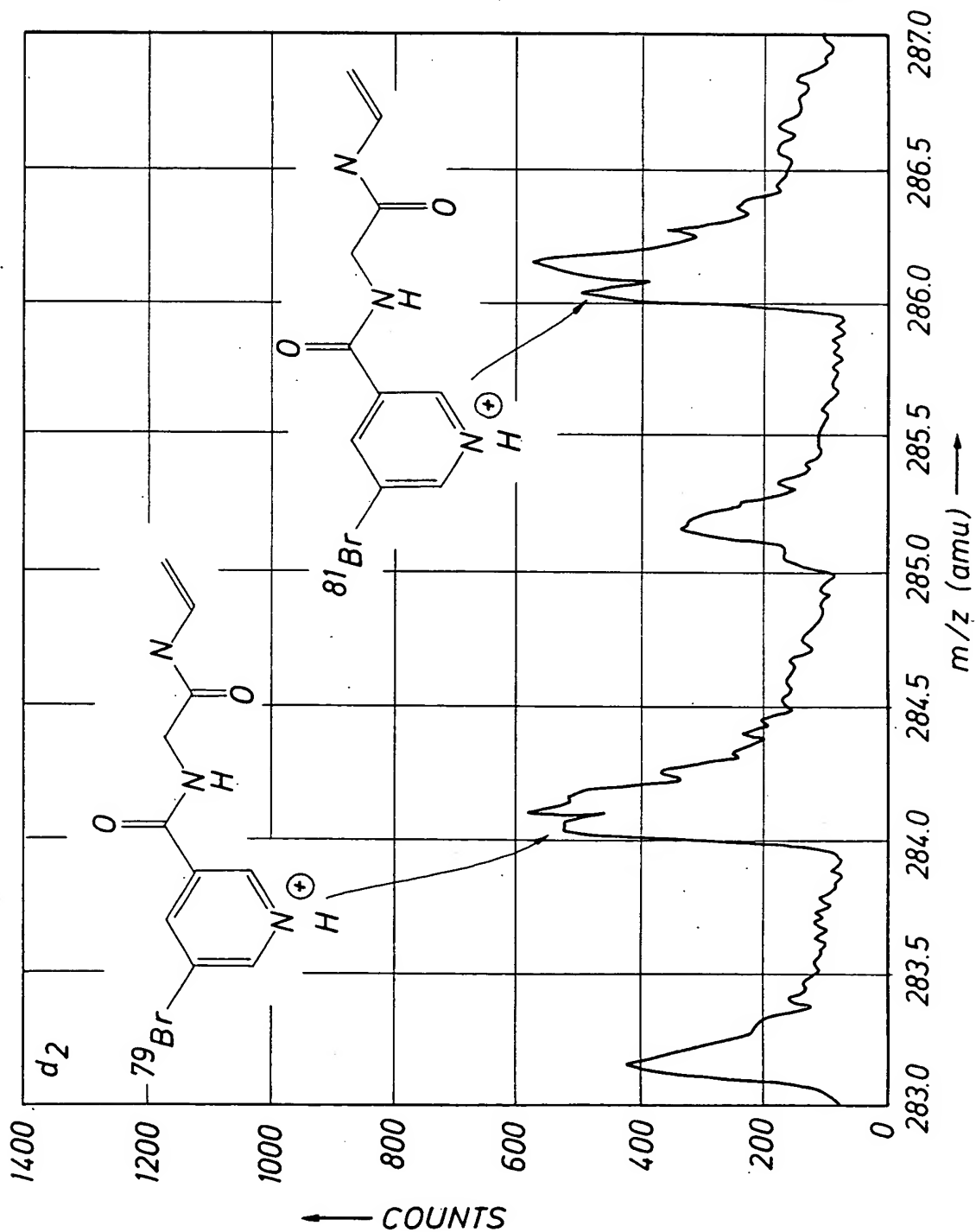
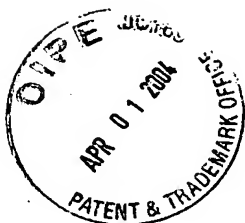


FIG. 30



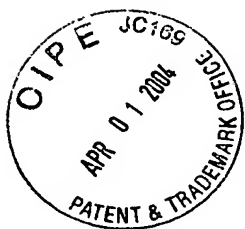
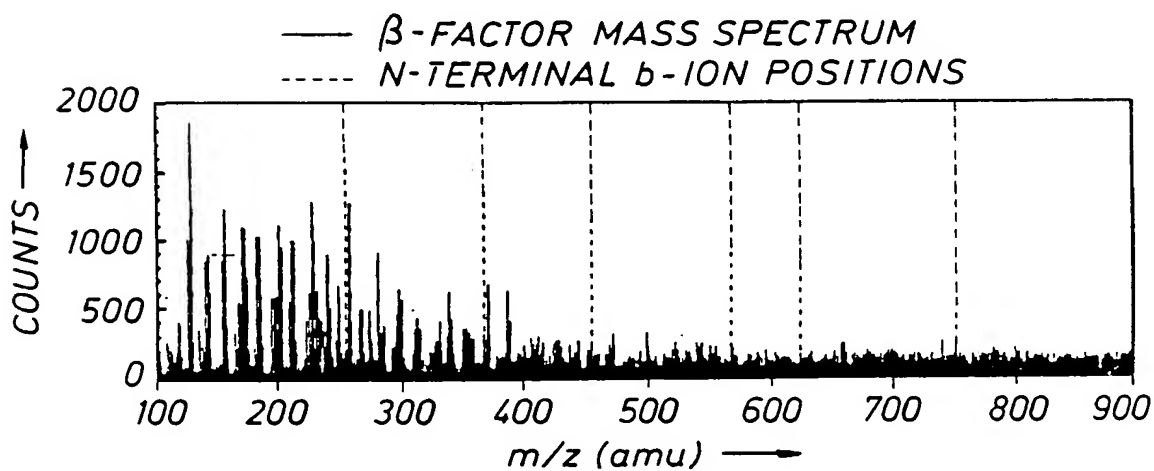
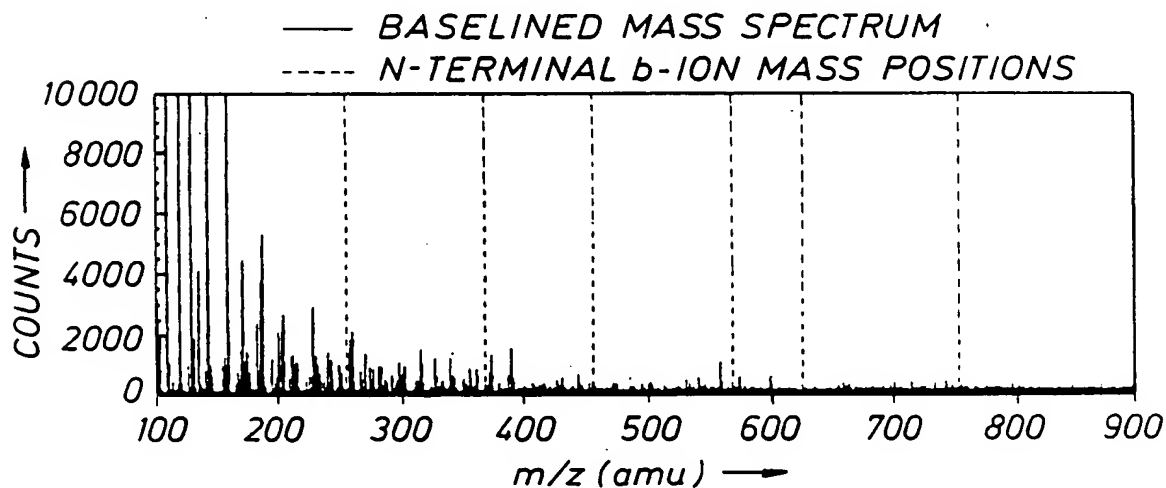
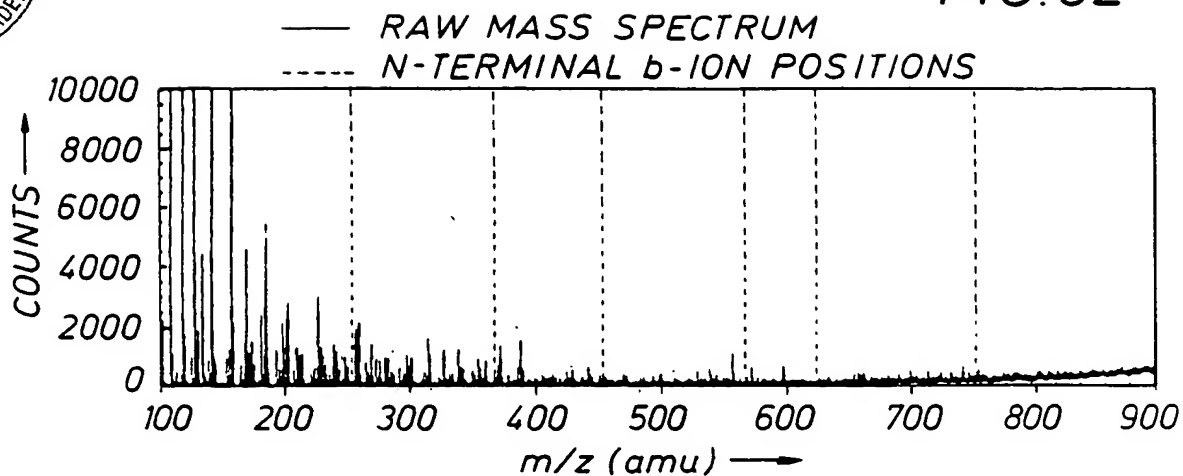


FIG. 32



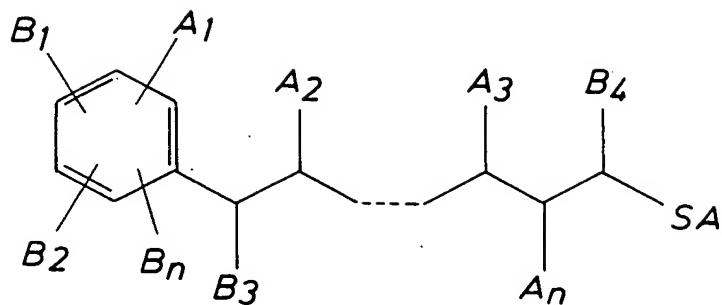
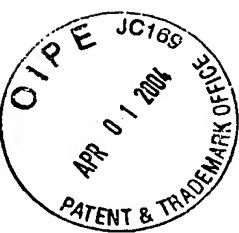


FIG. 34

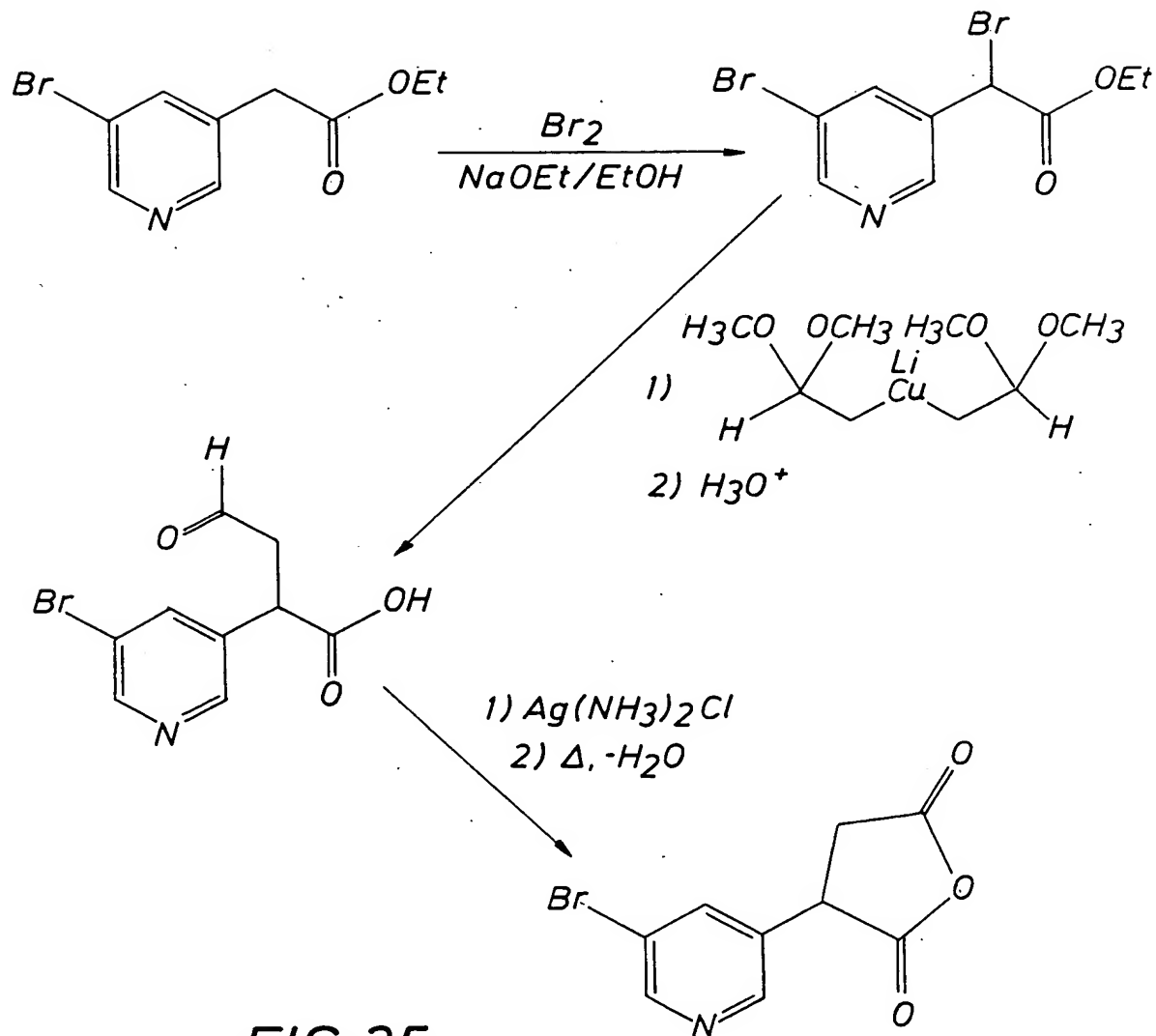


FIG. 35

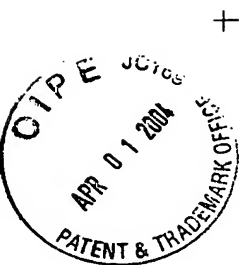
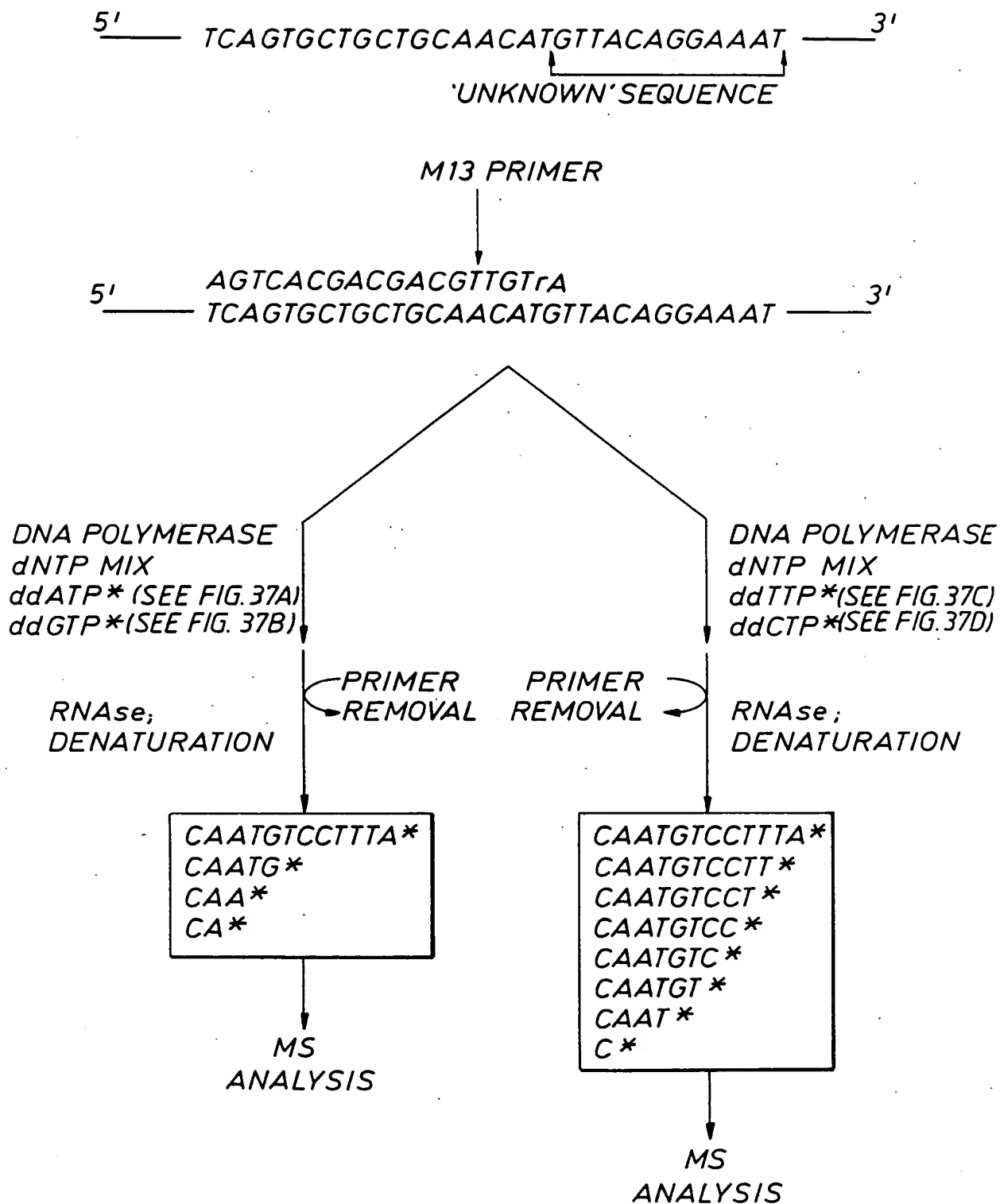
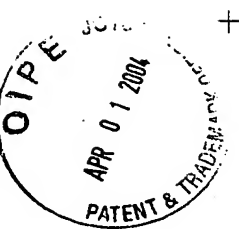


FIG. 36





ddATP*

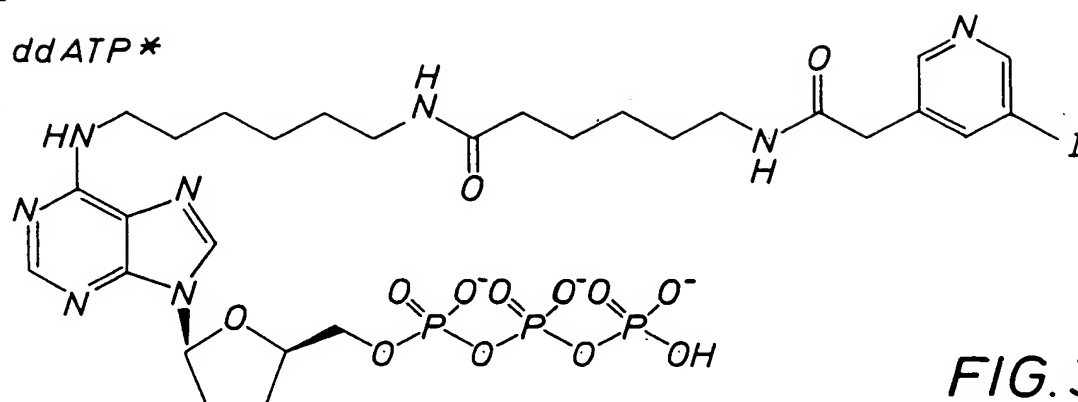


FIG. 37A

ddGTP*

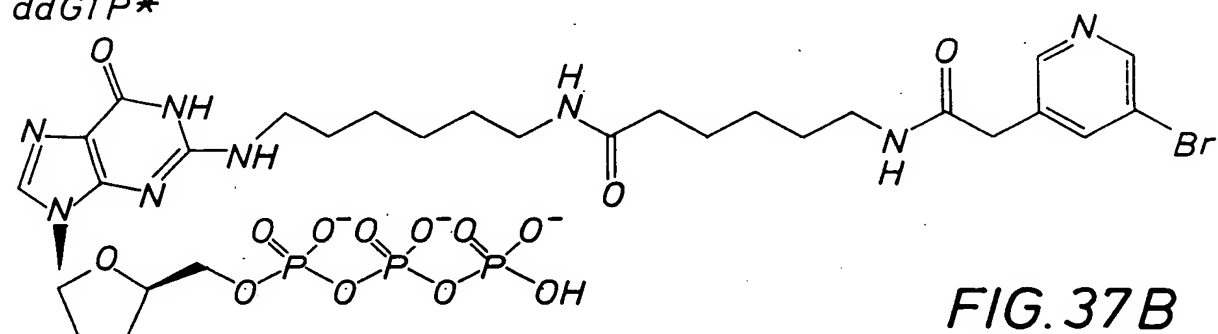


FIG. 37B

ddTTP*

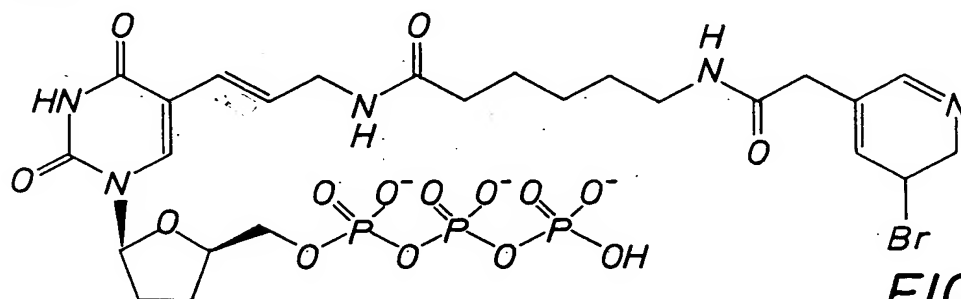


FIG. 37C

ddCTP*

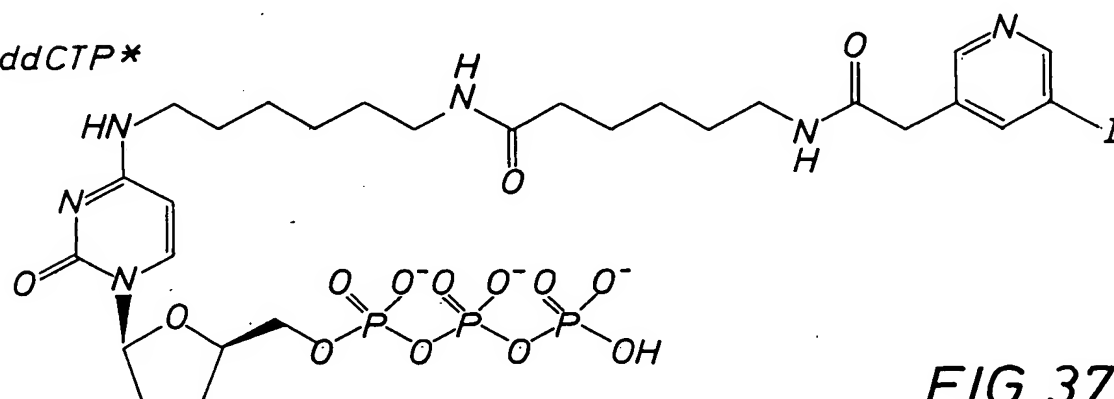
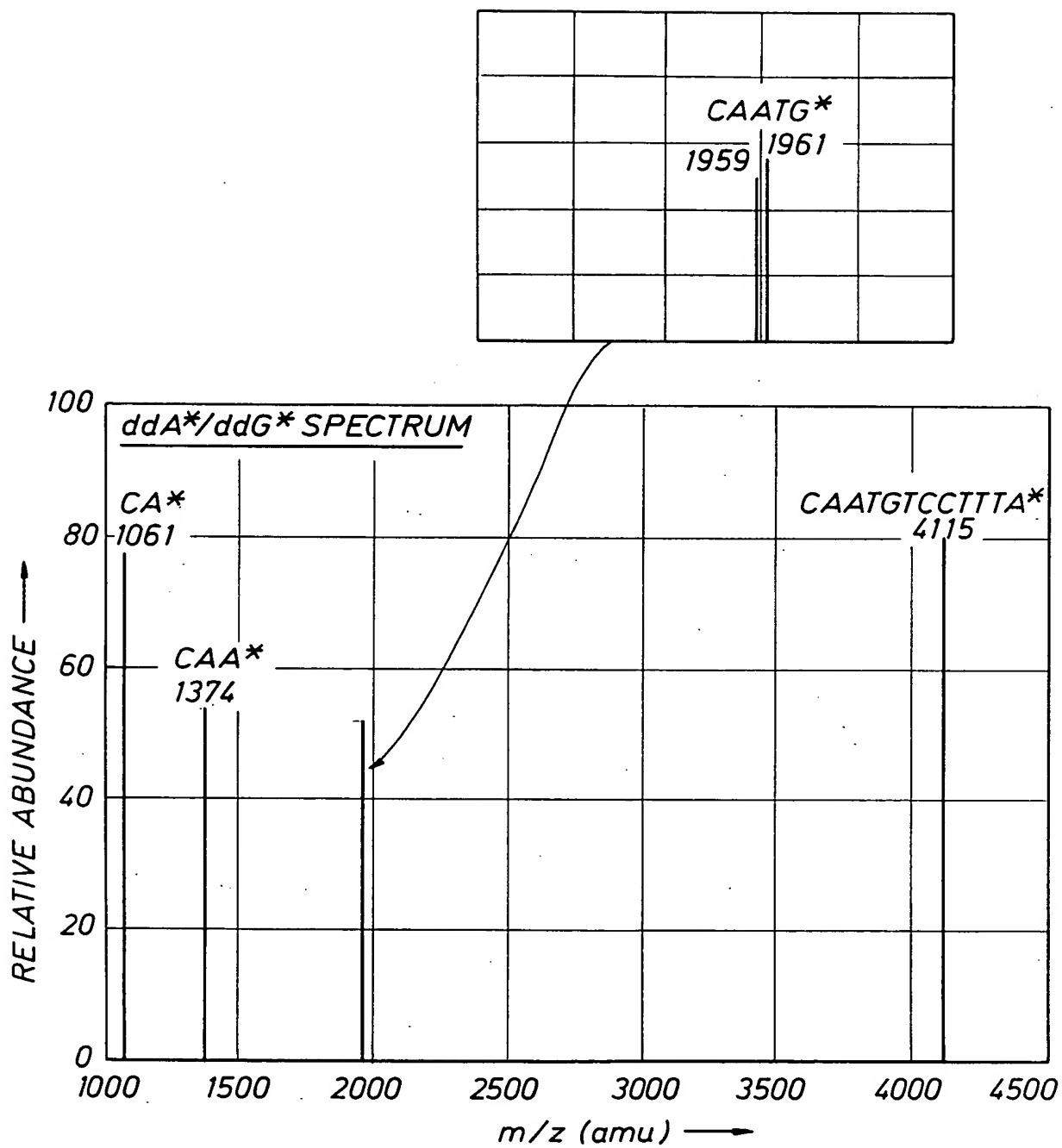


FIG. 37D



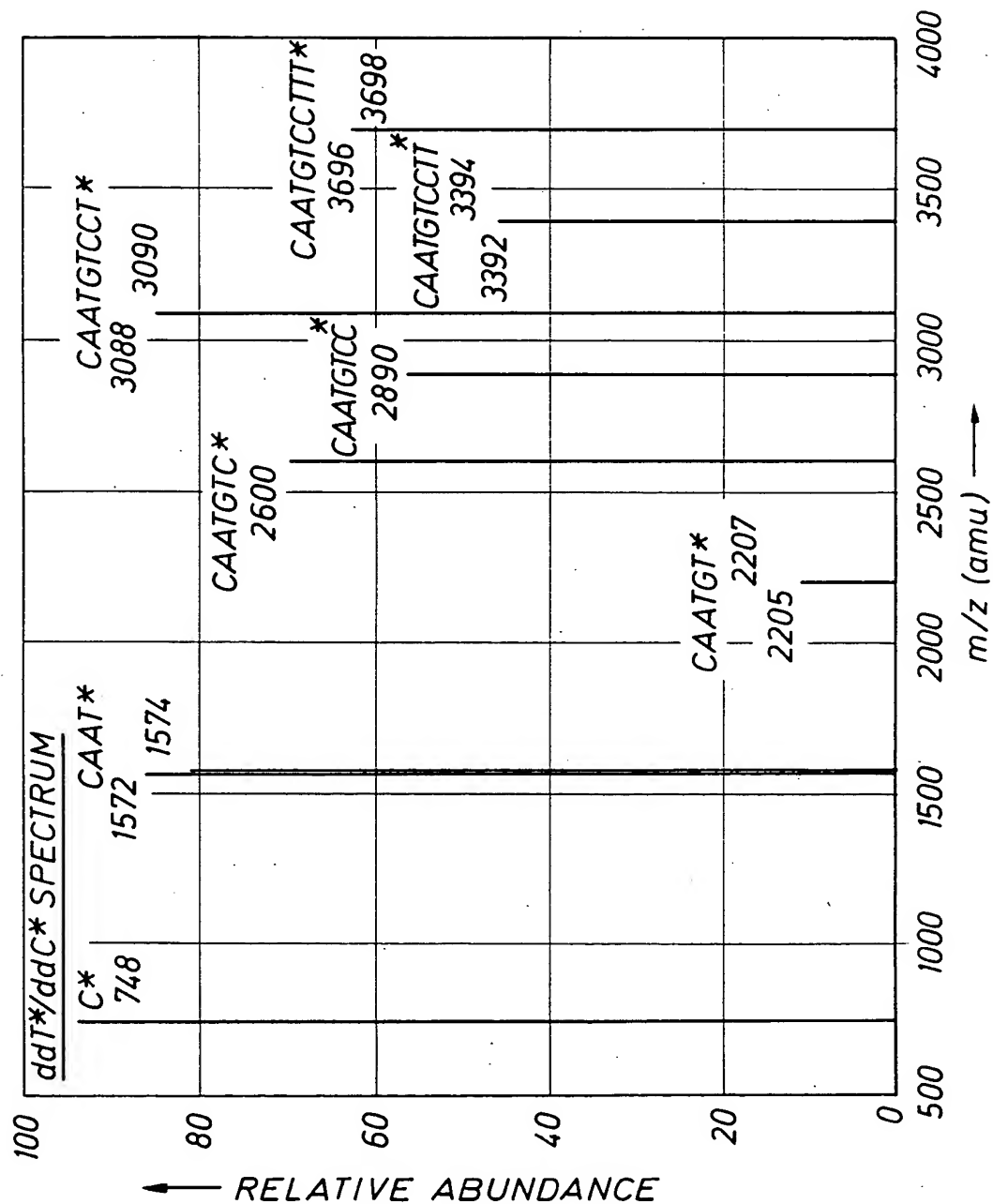


FIG. 39